Extract Dynamic Information To Improve Time Series Modeling:
a Case Study with Scientific Workflow

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Abstract—In modeling time series data, we often need to augment the existing data records to increase the modeling accuracy. In this work, we describe a number of techniques to extract dynamic information about the current state of a large scientific workflow, which could be generalized to other types of applications. The specific task to be modeled is the time needed for transferring a file from an experimental facility to a data center. The key idea of our approach is to find recent past data transfer events that match the current event in some ways. Tests showed that we could identify recent events matching some recorded properties and reduce the prediction error by about 12% compared to the similar models with only static features. We additionally explored an application specific technique to extract information about the data production process, and was able to reduce the average prediction error by 44%.

1. Introduction

Automated data collection and analysis has become the key tool to understand the world [20], [26]. We frequently encounter measurements in time, such as evolution of supernova [8] and gravitational wave [17]. In these cases, we often need to engineer new features to augment the existing data records in order to improve the modeling accuracy, for example, by including information from the most recent past data record [13], [39]. In general, feature engineering is a critical step in any data analysis tasks. Specific tasks for feature engineering could include organizing data into a convenient for the analysis platform, filling in the missing values, removing outliers, normalizing the values, as well as the above mentioned augmentation of data records. In this work, we explore a number of techniques to extract dynamic information to improve the prediction accuracy for a specific scientific workflow (to be described in more details in Section 2). However, we believe the majority of the techniques are easily applicable to other types of time series modeling efforts.

Time series data is a common output from automated data acquisition systems [7], [19], [31]. We broadly regard any data collection where each record contains a time stamp as a time series. This time stamp feature allows us to define a notion of time and compare data records according to their time stamps. Given any particular data record, we typically describe it as denoting the current event, a data record with a smaller value for its time stamp as an event in the past, and a data record with a larger time stamp value as an event in the future. A common goal of modeling a time series is to use the information about past events make predictions about the current event or future events. In this work we study the performance of transferring data from an experimental facility to a data center. We assume the performance prediction is made before the start of a file transfer, where the available information include all information about completed file transfers plus the static information already known about the current file to be transferred. How to best utilize the information about past information to improve the prediction accuracy is the main concern of this work.

Data scientists often spends a large fraction of their working day performing feature engineering tasks. Due to a large variety of possible tasks and lack of guidance on how to make effective choices, data scientists typically has to slowly and manually sift through the myriad of choices. There are a number of attempts to automate part of this process. For example, Brainwash is designed to automate many of the routine work and help data scientists to make choices more effectively [2]. Some work focuses on addressing feature engineering challenges in specific allocation domains [11], [14]. While others advocate for using deep learning to automate the selection of features [5], [14], [32]. In this work, we take advantage of the time stamps in data to develop techniques for time series data. These techniques can extract information from past history to approximate important relevant states of the system context not explicit captured by the data set. Tests show that our approach is quite effective in reducing the prediction errors.

Modeling of time series data also has its own unique
challenges. To determine the best model to fit a data set, one typically randomly select a sample of the data for training, testing and validation. This random shuffling of data is critical to avoid overfitting in selecting the appropriate modeling techniques and their associated parameters \[3, 4\]. However, this random shuffle is not appropriate for time series data because it does not preserve the time order. To avoid building a model on future data to test the past observations, we develop a nested cross validation \[6, 9\] approach that preserves time order.

In summary, the key contributions of this work include:

1) Develop a set of techniques to extract dynamic system information from recent past data records.
2) Design a time-order-preserving nested cross validation technique to determine the hyperparameters for the machine learning techniques examined.
3) Test our algorithms with a large set of performance monitoring data from a large scientific workflow. Tests show that our approach can significantly reduce the prediction errors.

This paper is partly based on the work previously reported by Yang et al. \[37\]. Their work primarily focused on demonstrating the capability to predict the data transfer performance for the application scientists. This paper focuses on the lessons we could learn on feature engineering. Furthermore, we have also conducted extensive tests with neural networks to automate the feature extraction process.

In the remaining of this paper, we give a description of the scientific workflow used as the test case in Section 2. We describe the efforts to augment the data records with recently completed events in Sections 4 and 5. A brief summary of lessons learned is given in Section 6. A brief summary of lessons learned is given in Section 7.

2. LCLS: a science use case

Our example time series come from monitoring the data transfer operations between the Linac Coherent Light Source (LCLS) and the offline compute facility both located at the SLAC, National Accelerator Laboratory. LCLS is a X-ray laser to create images of molecules, it is a basic tool for chemistry, biology, physics and materials. There are seven instruments with different detectors and X-ray beam characteristics that allow diverse types of experiments \[37\]. LCLS produces terabytes of data for each experiment. The current data pipeline involves two stages, the data files are temporarily stored at Fast Feedback (FFB) system, close to the experiment, and then to Analysis (ANA) system in the SLAC computing center. FFB provides fast, low latency access to the collected data. It is only used by the active experiments. ANA is large in size (4PB), shared between all experiments and holds the experimental data for many months. The data flow in shown in Figure 1.

When data is generated from an experiment, it is written to files on Data Storage Subnet (DSS) nodes via the data acquisition (DAQ) system. Multiple DSS nodes are used in parallel for each data collection (a run) and files from the same node constitute a stream. Typically 5-6 streams are run in parallel. A data mover then transfers files from DSS to FFB. The data is then transferred from FFB to ANA. The typical FFB transfer rate is limited by the rate the file is written to a DSS node, usually around 100-200MB/s. The typical limit for the ANA transfer rate in this process is about 350-400MB/s due to the speed of checksum calculation.

In this work, our aim is to use historical data from the LCLS workflow to build a model that can predict transfer rates of future transfers from DSS nodes to FFB and FFB to ANA. In particular, we conduct our analysis and model-building on a set of 258,765 transfers from May 2017 to January 2018 where 131,274 transfers take place from DSS to FFB and the remaining 127,491 are from FFB to ANA.

LCLS has seven instrumental stations with different types of detectors. The stations are distributed in two buildings known as the Near Experiment Hall (NEH) and the Far Experiment Hall (FEH), see Table 1. Due to this physical separation, these instruments are also attached to different local file systems. Table 1 has the number of files produced by each of the seven instruments used in the data collection. From this table we see that cxi, xpp and mec are used much more than the others. The overview of statistics on transfer rate and file size in FFB and ANA transfers are shown in Figure 2.

Next, we describe the file generation and transport process to give more information about what features are important to predicting the file transfer performance.

File Size. Based on the past experience, the performance of a file transfer is heavily dependent on the file size. The first feature we plan to explore is the file size. Figure 3 shows the distribution of the file sizes and transfer rates.
### TABLE 2. SUMMARY OF LCLS DETECTORS: INSTRUMENTS IN THE TOP ROW ARE LOCATED IN NEAR EXPERIMENT HALL (NEH) AND THOSE IN THE BOTTOM ROW ARE LOCATED IN THE FAR EXPeriment HALL (FEH).

| Instrument | FFB File System | DSS → FFB Host | FFB → ANA Host |
|------------|----------------|----------------|----------------|
| amo, srx, spp | ffb11            | psana\{102,103\} | psana\{102,103\}, psexport\{01,02,05,06,07,08\} |
| cxi, mec, mfx, xcs | ffb21            | psana\{201,202,203\} | psana\{201,203\}, psexport\{01,02,05,06,07,08\} |

| STATS | size (gigabyte) | transfer rate (MB/s) |
|-------|-----------------|----------------------|
| median | 4.0             | 47.9                 |
| mean  | 13.8            | 81.2                 |
| std   | 22.1            | 91.0                 |
| min   | 0               | 0                    |
| max   | 1304.14         | 498.2                |

(a) Histogram of transfer rate (to FFB)
(b) Histogram of file size

Figure 3. On the whole, ‘cxi’ and ‘amo’ tend to have faster transfer rates, while ‘mec’ has the slowest transfer rates.

We see that different instruments have clearly distinctive distributions.

Nodes and Streams. As data is generated from an experiment, it is written in parallel streams with each stream assigned to one DSS node. This data is then simultaneously written to the FFB by the data mover/host. Once a file for a stream reaches a cap of 100GB, which is configurable, the file is closed and a new file for the same stream is opened. We call a set of files for the same stream chunks. The structure of chunks and streams are embedded in the file name and have to be extracted. Such information allows us to better understand the data transport process and make more accurate predictions.

In Figure 4, we plot the transfer rate over time for all nodes of instrument ‘xpp,’ and we can see that different nodes are dormant and active during different parts of the year.

File systems. From the data overview in Table 2, we also notice the close relationship between instrument and FFB file system, which is the source file system in the ANA transfer process. Therefore, we expect this source file system also affects the transfer rate, and we show the distribution plots of the two different source file systems in Figure 5.

Delayed Transfers. Different streams of a chunk are transferred at the same time, but there are instances where a stream’s start time is significantly later than the start time of the first stream in the same chunk. One example of this is in Table 3 from chunk 00 of experiment ‘e991-r0002’ on instrument ‘mfx’. We see that the first two transfers are almost 3 hours before the later two streams. The difference in target hosts suggests that there may have been a problem with psana203 during this time. A slightly more nuanced example is in Table 4. We see that the first two streams start at the same time, then there is about a 2 minute gap in subsequent streams. This leads to a slight bump in transfer rate. Similar to above, we see that the target host is different between the first two streams and the latter three.

From Figure 6, we clearly see the impact of the start time difference, especially when the start time difference is large. On the other hand, if the difference is on the order of a few minutes, then the pattern is less clear.
3. Modeling LCLS Data Transfer Performance

In this section, we briefly review the main modeling approaches we will be using to evaluate our feature engineering methods. In addition, we will also outline our cross validation procedure that respects time order of the time series data, and establish a base line for evaluating the effectiveness of the feature engineering efforts.

There is a significant amount of published work on modeling time series data, we refer to the interested readers to books and reviews on this subject matter for a comprehensive treatment [7], [22], [30], [31], [34]. For this work, we have chosen to use a few common decision tree based modeling approaches because they have high quality software implementations that are freely available to us, and are efficient to compute. Additionally, they are known to be effective in prediction, to produce interpretable results, and to require a relatively small amount of hyperparameter tuning [16], [23], [38]. In particular, we have selected to use an implementation of random forest [29] and a number of gradient boosting techniques [15], [10]. We will also be exploring a few variations of neural networks in Section 5. Despite their popularity, we found there are simply too many ways to construct different neural networks and we have not been able to find the best variant for our prediction task. For this reason, we will be mostly staying with decision tree based prediction models.

Order-preserving Nested Cross Validation. For each modeling method, we tune the hyperparameters using nested cross validation (CV) for time series, as described in Algorithm 1. This nested CV preserves the time order of the data records and prevents information leaking from the training set to the validation set. It guarantees this by having each element in the training set precede each element in the validation set during each iteration. This type of cross validation is important since we are using lagged features to predict future transfer rates. We measure the performance based on Root Mean Square Error (RMSE) in this process.

Baseline model with static features. Now that we have selected the class of methods for constructing the prediction models, the key next step is to choose the features to be used for the models. The first set of features contains 22 fields from the given performance monitoring data set. These features are known before the start of the file transfer and called static features for the purpose of this modeling exercise. These features include:

A: file size, instrument, experiment number, target host, target file system, and source storage system.

Among these features, instrument, source file system and target file system are encoded using one-hot encoding, and experiment number is treated as categorical values. With a good amount of exploration of the hyperparameter space and different decision tree based modeling methods, the best of our tree-based modeling approach turned out to be XGboost, and it gives a RMSE of 64.3 MB/s when we use the first 90% of the time series as training and last 10% of the time series for testing.

From the feature importance matrix in Table 5 which only displays the 5 most important features, we notice that file size is the dominant factor affecting the transfer rate, and experiment number also has large importance on the transfer rate. The instruments, all seven of them together, count for approximately 10%, which make it the third most important in predicting transfer rates. Among the instruments, cxi is
Dynamic Features: Time Lags

The previous model with the static features uses only the information from the current event at time \( i \). In statistical techniques for time series modeling, we often use information from time \( i-1, i-2, \) and so on \([19, 23]\). These most recent past data records are also called lags because they have a fixed amount of lags in time (index) dimension. We typically refer to the data record at time \( i-1 \) as lag 1 of the data record at time \( i \), similarly, the record at time \( i-2 \) is lag 2, and record at time \( i-\ell \) is lag \( \ell \). Next, we consider taking information from some of these lags to augment the feature set used in our tree based models. One important caveat to note here is that the most important piece of information from these past events are their data transfer rates. In order for the data transfer rates to be available, these past events have completed before the current event (\( i \)) starts.

The standard method of select information from the past is based on time alone. However, since our time series has a number of different attributes/features, we can define different types of lags based on the features other than time. For example, since each LCLS experiment has its own specially image capturing device and its own dedicated storage system, how quickly the last completed file transfer would be strongly correlated with the speed of current file transfer. This is because the two file transfers share many common systems. The information from the recent past event, i.e., the lag, could be highly useful for predicting the performance of the current file transfer.

After some exploration, we define five different types of lag variables. Four of them share the same instrument, experiment, source file system or target file system with the current event. In other words, these lag variable are generated by taking the value from the most recently finished job on the same instrument, experiment, source file system or target file system. Because instrument, experiment, source file system and target file system are all known information from the data record at time \( i \), the most recently completed events with these information are easily identifiable with suitable preprocessing. The fifth one takes the value from the most recently finished job, i.e., considering the time alone. There are some correlations between these lag variables. For example, transfer rate from the most recently finished job on the same instrument is highly likely to be the same as that in the same experiment.

We are not only interested in lag 1, but also lags beyond the first one.

After an extensive amount of cross validation, we choose add to the static features the following set of dynamic features based on the lags with different properties.

| Feature | Importance |
|---------|------------|
| File Size | 66.82% |
| experiment number | 17.32% |
| cxi(instrument) | 6.15% |
| fll(source file system) | 4.85% |
| mfx(instrument) | 2.60% |

### TABLE 5: Feature Importance According to XGBoost with Static Features.

the most influential, presumably, it is the most frequently used instrument, as shown in Table 1.

4. Dynamic Features: Time Lags

We have tested the performance of many combination decision trees and their hyperparameter values. Figure 7 shows a sample of the prediction results plotted against the actual observed performance. From this set of tests, we see that the Gradient Boosting method achieved the smallest RMSE overall. By using the parameters: learning rate = 0.1, n estimators = 600, max features = 4.12, max depth = 11, min samples split = 700, min samples leaf = 10, the Gradient Boosting method achieved RMSE of 56.9MB/s, which is about 12% less than the RMSE achieved with the static features in Group A.

The new feature importance for the tuned Gradient Boosting Tree is shown in Table 6. Comparing Table 5 with Table 6, we can see the importance of file size decreases with the lag variables, which indicates the lag variables are indeed contributing to transfer rate prediction.

In Tables 3 and 4, we showed two cases where large gaps between start of what otherwise might be consecutive...
files could indicate significant performance variations. The presence of the variable “time difference between same experiment” in Table 6 is thus expected. However, the differences between Tables 3 and 4 suggest that further investigation is needed.

5. Automatic Feature Discovery with Neural Networks

From the feature engineering work presented in the previous sections, we can confirm that constructing a complete feature set is a challenging and tedious work. For example, the dynamic features is Group B1 are chosen after pretty extensive set of cross validation runs, however, there is no guarantee that our exploration were complete in any way. Inspired by a number of reported effort on using neural networks to automate the feature selection process [1], [11], [14], [24], [28], we next proceed to explore how neural networks might be used to reduce the effort of manual exploration. Some of the key characteristics of neural network include its ability to learn the complicated non-linear interactions among the input features and to produce new features to represent these interactions. In this work, we plan to explore three different neural network architectures that extract different types of information from time series. The first one only has fully connected layers, which is considered a general-purpose basic architecture [12], the second one includes convolutional layers, which use convolution to extract trends in time series [27], [28], and the last one uses a long short term memory (LSTM) model, which is a pure auto-regression process designed to model complex time series based [21], [18], [35], [33]. In addition, we design a different selection of features from the current and past data transfer events for each of the three different neural networks. To take advantage of the neural networks as a feature generation mechanism, we also explore combining the intermediate outputs from these neural networks to generate an ensemble network. Tests show that this ensemble network is able to achieve the best prediction accuracy on average.

Next, we first describe the construction of these four neural networks and their input features, and then describe how they perform.

5.1. Neural Network Structures and Their Input Features

The first neural network model implemented is a 3-layer fully connected model, see Figure 8. In terms of input features for this neural network, we plan to use the last set described in the proceeding section. We add two features about date and time as well as the concurrency levels of the file transfer activities 1. These features are selected due to their potential to represent daily and weekly network traffic patterns as well potential for network traffic congestions. Altogether, we have the following set of features as input to the

A: file size, instrument, experiment number, target host, target file system, and source storage system.
B: day of week, hour of day.
C1: number of active file transfers from the same experiment, number of active file transfers from the same instrument.

1. These features are not explicitly present in the original recorded values, but can be extracted through know procedures: for example the time of day and data of week can be extracted from the unix time stamp representing the start time, and the concurrencies could be computed by examining the start and end time values of file transfers. Note that these procedures do not require any domain knowledge about the specific scientific workflow.
D1: transfer rates and time differences of Lag 1 on the same instrument, experiment, source file system or destination file system; transfer rate of lag 1 and Lag 5 in time alone.

As in the previous models, the categorical variables are converted into one-hot-encoding variables.

The second neural network architecture we explored is the Convolutional Neural Network (CNN) [27], [28]. CNN applies the mathematical operation known as convolution to extract features at different scales. This operation is very effective at discovering the local information and relationship among the neighbor features. In this particular application of predicting file transfer performance, one critical information we need to infer is the status of the data network carrying out the next file transfer. As in most time series modeling tasks, we believe the state of the data network could be approximated through the performance of the recent data transfers. We believe that it does not make sense to take a convolution over different features, and plan to only apply convolution over time. In order for the convolution operation to extract useful information we need to provide enough information from the recent past. We take 20 lag variables for each file transfer record, and each lag variable is obtained from the most recently finished file transfer belonging to the same experiment. Altogether, the full list of input features includes:

A: file size, instrument, experiment number, target host, target file system, and source storage system.
B: day of week, hour of day.
C1: number of active file transfers from the same experiment, number of active file transfers from the same instrument.
D2: transfer rates of Lag 1–20 from the same experiment.

Following the convolution layer, the activation function used is ReLU and a MaxPool layer is followed after each CONV net. The overall architecture of our CNN model is shown in Figure 9.

The third neural network architecture we explore is Long Short-Term Memory (LSTM) [21]. LSTM is a recurrent neural network that uses the information from the current time step as well as recent past information to make predictions. This is especially well-suited for time series data because it learns to store information over extended time intervals by recurrent backpropagation. We can regard LSTM as automatically discovering the dynamic lag features, we only need to include the static features as input features. The number of LSTM layers can be thought of the mechanism for remembering past time steps. In this case, we found two to four layers of LSTM work quite well. In our tests, we found the five Lag 1 defined in Group D1 are useful as input and we include all static features for each these five past events along with their transfer rates and time differences mentioned in the definition of Group D1.

If we only use the past information, then we will be missing the static features of the current data transfer as input feature. To make the data record about the current event match the structure of the past events, we add the average of the transfer rates from the past five events in Group D1 as the expected transfer rate for the current event. In later discussions, this set of features is referred to as the projected performance.

Following the LSTM layers, we have added one or more fully connected layers before the final prediction. In this regard, we can think of LSTM layers and the fully connected layers as creating features for the final prediction.

The above three neural networks all ends with a fully connected layer to produce the final output, we regard this final fully connected layer as performing final combination of the intermediate features extracted by the neural networks, and the input to this final layer as the final features extracted. The fourth model is an ensemble model that makes use of all these final intermediate features. We have conducted a number of different tests on combining the models, and eventually choose to use the combination shown in Figure 10.

To select the hyperparameters for the neural networks mentioned above, we use Adam [25] with mean square error (MSE) of predictions as the loss function. Each of the four models are tuned separately.

5.2. Test Results with Neural Network Models

In our experiments with the fully connected model, we have explored a number of different variations by adding regularization, dropout layer and step-dependent learning rate. Our tests show that the L2 regularization does not reduce the average prediction error with the 3-layer fully connected model. Similarly, the strategy of dropping out some links also increases prediction error, most likely because our model is relatively simple and there is no links to drop. We find adjusting the learning rate based on the step count could reduce the average prediction error noticeable.
After extensive cross validation and optimization with Adam, we find that a learning rate of $10^{-3}$ and hidden layer size of 250 (for both hidden layers) give the best validation loss. We adjust the learning as follows: (1) start with the initial learning rate ($10^{-3}$); (2) if the loss has not decreased in 40 epochs, then reduce the learning rate by a factor of 0.1; (3) use the same learning rate for no more than 120 epochs before reducing it by 0.1. Applying this model to the test dataset, we obtain a RMSE of 71.48MB/s.

With the CNN model, similarly experimented with different learning rate, hidden layer size, filter size, convolution window size, and so on. The smallest loss is achieved with learning rate = $10^{-3}$, hidden layer size = 128, filter size 1 = 3, filter size 2 = 3, filter num 1 = 32, filter num 2 = 16. The resulting RMSE on test data is 76.01MB/s.

For the LSTM model, there are also many ways we can tweak the model and architecture. We have presented some of the best results in Table 7, indicating that using a relatively larger hidden size of LSTM layer can increase the model complexity and encourage the model to learn more from the features. Besides of that, adding the static features of the current transfer can increase the prediction accuracy.

We finally take the best hyper-parameters and network architectures from each of the model to form an ensemble model, see Figure 10. We take the intermediate feature outputs after the fully connected layer in each model, and ensemble the feature outputs together to form the new feature set. The ensemble features are then trained through a two-layer fully connected model. After some additional optimization with Adam, this ensemble model achieves RMSE of 59.8MB/s.

**6. Dynamic Features: Incorporating Data Management Details**

Section 2 has a description of the variables captured by the performance monitoring system at LCLS. In the previous modeling exercises, these variables are used as static features labeled as Group A. There are two exceptions. The first exception is the Unix time stamp for start time, which is digested into a couple of different features in Group B used in the previous models. The second exception is the file name of the data file being transferred, which has not been used so far. Since the file name is unique for each file, we were not sure how to make use of it until we notice that the file name is composed of the experiment, chunk, stream, and a sequence number with the stream, see more discussion in Section 2. The data acquisition system of LCLS composes these file names use a numerical representation of these properties about the physical experiment. Even though such information is specific to LCLS, however, we can imagine that the automated data collection system would similarly compose data file names based on unique attributes of the data collection process so as to ensure the file names are unique.

Among the features that could be extracted from the file names, the experiment number and the chunk number are already explicitly recorded by the performance monitoring system. The new features are the stream number and the sequence number (within a stream). Next, we describe our attempt to make use these new features to further improve the prediction accuracy.

Based on the previous experiences and with some additional explorations, we decided to expand the list of features as follows: (1) Expand Group C1 with additional measures of concurrency for target storage systems to form a new Group C2. These features should better reflect the workload on the target storage systems. (2) Expand Group D1 with additional information both on the source storage system as well as the target of the file transfer to form a new Group D3. This change is designed to capture the status of both storage systems involved in a file transfer. Through extensive testing, we decided to only include information from the most recently completed file transfers with the same experiment number and so on. This is an expansion of the previous defined Group D1, with fewer lags than used in Group D2.

(3) Based on the examples shown in Tables 5 and 6, we expect the time differences between start of a file transfer in a stream has significant impact on the actual data transfer rate, even if the mechanisms for the relation is not obviously visible. Such information could be extracted once we figure out how to digest the file names to identify the streams and sequence within a stream. This time difference within a stream is captured in a new feature group E.

In summary, we have the following feature set as input to next prediction models:

- A: file size, instrument, experiment number, target host, target file system, and source storage system.
- B: day of week, hour of day.
- C2: Number of total jobs and number of unique experiments running on the same target file system, target host, and node, respectively, when the current job is started.
- D3: Statistics (transfer rate, file size, time between last job’s stop time and current job’s start time) from the last job on the same instrument, target file system, target host, target node, experiment, and chunk, respectively.
- E: Time difference between the start time of the first job of the chunk and the start time of the current job.

**Random Forest Results.** Using the nested CV algorithm with the training set $X$ equal to the first 90% of the rows, $k = 10$, $train\_width = 20000$, $train\_size = 5000$, $test\_width = 2000$, $test\_size = 500$, we then retrain the random forest model using the best hyperparameters on a 30000 row subset of the first 90% of the rows of $X$, and evaluate RMSE on a 3000 row subset of the last 10% of

2. The end time is considered as unknown or to be predicted, therefore, not usable as input to the modeling procedures.

3. We were hoping LSTM would automatically identify the most important features from Group D2. Unfortunately, additional exploration is needed to ensure this automatic process could produce more accurate models.
The rows of $X$, where the prediction is $\max(0, \text{prediction})$. This yields an RMSE of 52.8 MB/s.

A scatter plot of the actual versus predicted transfer rates is shown in Figure 11 and the most important features are given in Table 8.

**Xgboost Results.** Using the nested CV algorithm with the training set $X$ equal to the first 90% of the rows, $k = 10$, $train\_width = 2000$, $train\_size = 6000$, $test\_width = 2000$, $test\_size = 800$, we then retrain the Xgboost model using the best hyperparameters on the same 30,000 row subset as the random forest, and evaluate the RMSE on the same 3000 row subset as the random forest, where again the prediction is $\max(0, \text{Xgboost prediction})$. This yields an RMSE of 36.1 MB/s.

A scatter plot of the actual versus predicted transfer rates is shown in Figure 12 and the most important features for this model is listed in Table 9.

**Observations.** On the question of which features are the most important for the prediction models, we see one common trend from Tables 5, 6, 8, and 9 that is, the performance of the most recently completed data transfers is highly influential in predicting the current file transfer performance, especially the last event, also known as Lag 1, on the same data path, because these data transfer events share the same source storage system, the same communication network, and the same target storage system. When the Lag 1 has just completed recently, we can expect the current file transfer to have the same performance, because the current state of the systems involved in the data transfer must be similar to that the just completed one. Given this general observation, the key objective of our feature engineering task would be to discover the best way to represent the current status of the system by teasing out condition that is most
similar to the current event. This is a general lesson that is applicable to many application scenarios.

Even though we started out this section with the extraction of application specific information from file names, i.e., the stream number and the sequence number within a stream, however, the feature importance results from the actual modeling exercises, see Tables 4 and 9, indicate that these application specific features are not particularly important, none of the application specific features made to the top of the feature importance lists. Therefore, we may not need to find the most perfect match when identifying the lag variable. We would have expected the more accurately a lag event matches with the current event the more similar the performance, however, the actually underlying systems are influenced by more variables than is captured by the monitoring system, therefore, even if we can match all the features we know of, there is no guarantee that the two events would actually be perfectly matched. Furthermore, the more specific is the matching condition, the fewer events would satisfy, which would lead to more records with no matching past event or stale matches from far past where the states of the systems are not comparable any more.

We also see significant difference among the feature importance tables, which suggests that we have yet found a definitive set of features that would best model the particular time series. Additional work is need to verify whether there are better ways to construct a feature set. For the moment, we advise readers to include more variety of features. Since the models including feature group D3 achieved lower RMSE, we believe the feature group D3 is better than D1 and D2. Even the group D2 contains more variables, the group D3 has more variety, which we believe is key to its success.

7. Summary

When analyzing time series data, we often face the situation where some features related to the key objective are missing from the existing measurements. For example, in our task of predicting the file transfer performance, we would ideal know exactly how busy are the source storage system, the data communication network, and the target storage system, however, such information is missing from the performance monitoring data we have access to. In this situation, we could extract proxy information from the recent past records. In this work, we explore three approaches to extract such dynamic information from a set of network data transfers from a large experimental facility and data center. We first try to use a fixed number of recent past records (also called lags), an approach is applicable to any time series data. We find that these dynamic features are able to reduce the average prediction error by about 12%, using the same Gradient Boosting Trees that was also used to model the data transfer performance with only static features in the raw data. Our second approach utilizes neural networks of various configurations to automatically extract key features from recent past data records. Even though this approach was successfully used in the literature, we were unable to find a neural network that was more accurate than the Gradient Boosting Trees. Finally, we explored an application specific technique that took advantage of the information embedded in the file names to identify recent past data records involving the same compute, storage, and network systems. This set of application specific features allowed us to build a more accurate Gradient Boosting Trees, where the prediction error was reduced to 36.1, a 44% reduction compared with the original model with static features.

Since our approach augment the time series data with information from the past, it is critical that we avoid leaking information among the data sets for training, testing, and validation. In this work, we designed a nest cross validation approach that guarantees to prevent this leakage. We believe that this algorithm is key to selecting the approach hyperparameters for our machine learning models.

For future studies, we plan to study the propose nest cross validation algorithm more carefully. Even though we believed the application specific information was critical to the success of the final feature set presented in Section 6, the feature importance information from the actual models does not agree with our expectation. It would be worthwhile to examine this discrepancy further. In addition, we believe the neural network approach has great potential despite our current inability to make an effective use. For example, our current training data range might be too narrow or too wide, by adjusting this training data range, we might be able to capture the most relevant trends and improve the prediction accuracy.

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