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Tool Resource Prediction for Genomic Datasets

Masterproject Report

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Contents

1 Introduction

Galaxy (at https://galaxyproject.org) is a web-based, open-source scientific analysis platform designed to analyze large biomedical datasets commonly found in genomics, proteomics, metabolomics, and imaging [5]. For this, researchers can access more than 5500 tools provided by the Galaxy ToolShed. Galaxy's graphical web interface enables even users without programming background to use sophisticated and powerful tools for various tasks in the field of bioinformatics in a visual and interactive way.

Currently, Galaxy allocates and provides a fixed amount of memory for each tool. This can result in over- or under-allocation of memory. As a consequence, jobs run with a particular tool may fail because there is not sufficient RAM for its usage, or resources may be wasted as the actual memory usage is much less than the space allocated by Galaxy.

The amount of CPU, RAM, and processing time a tool takes to finish is dependent on the input dataset size and the computational complexity of the tool. By examining data which got recorded on the European instance of Galaxy (https://usegalaxy.eu), the goal of this work is to evaluate different Machine Learning methods to predict the future memory usage of tools based on the size of the input data and other extractable content.

This report first explains some theoretical basics of Machine Learning methods (chapter 2), after which it discusses works that had similar approaches and contents (chapter 3). Then, the concrete methods and applications of the dataset and models are explained (chapter 4), which are further evaluated and assessed in chapter 5. Finally the findings of the project are discussed and future research possibilities are brought forward in chapter 6.

2 Background

2.1 Random Forest

Random Forest is a commonly used supervised machine learning algorithm for classification and regression problems. It was first introduced properly by Breiman in 2001 [9]. A Random Forest is categorized as an ensemble learning algorithm, since it is constructed of multiple decision trees (see Figure 2.1).

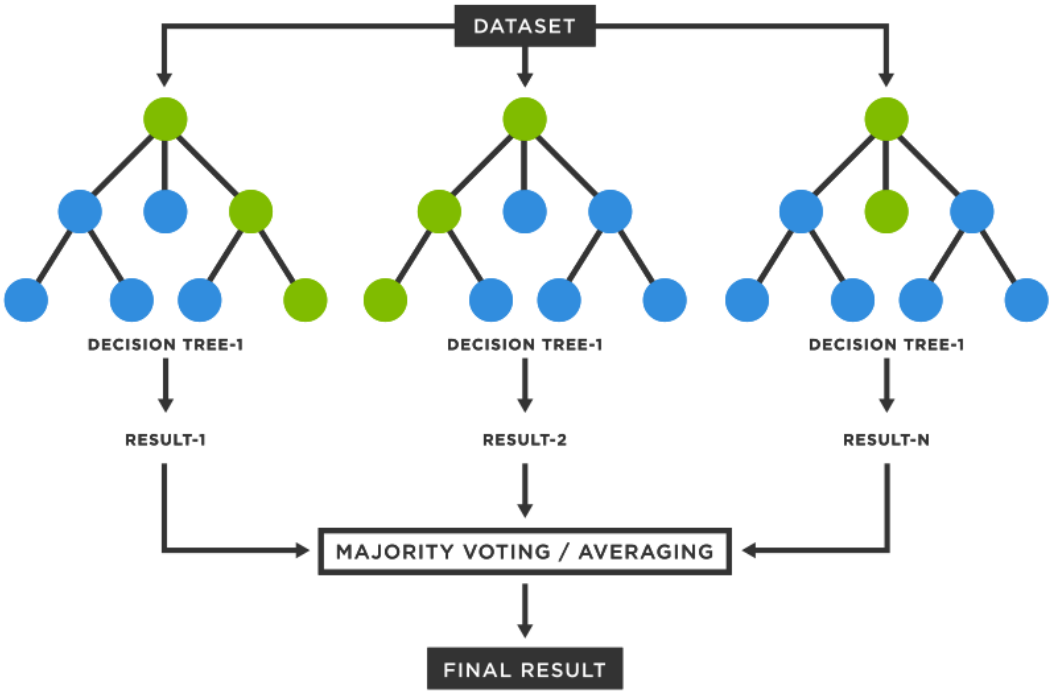

Figure 2.1: Structure of a Random Forest consisting of multiple decision trees (source: [2])

A Decision Tree learns to predict a target feature by inferring simple decision rules from the dataset. It is comprised by a series of decision nodes, branches and leaves. Each decision node in the tree questions the data and splits it into two branches aiming to maximize the information gain by doing so [21]. A prediction can be done by starting at the root node and following the decisions until a leaf node is reached, which gives the output of the tree. An example of such a tree can be seen in Figure 2.2.

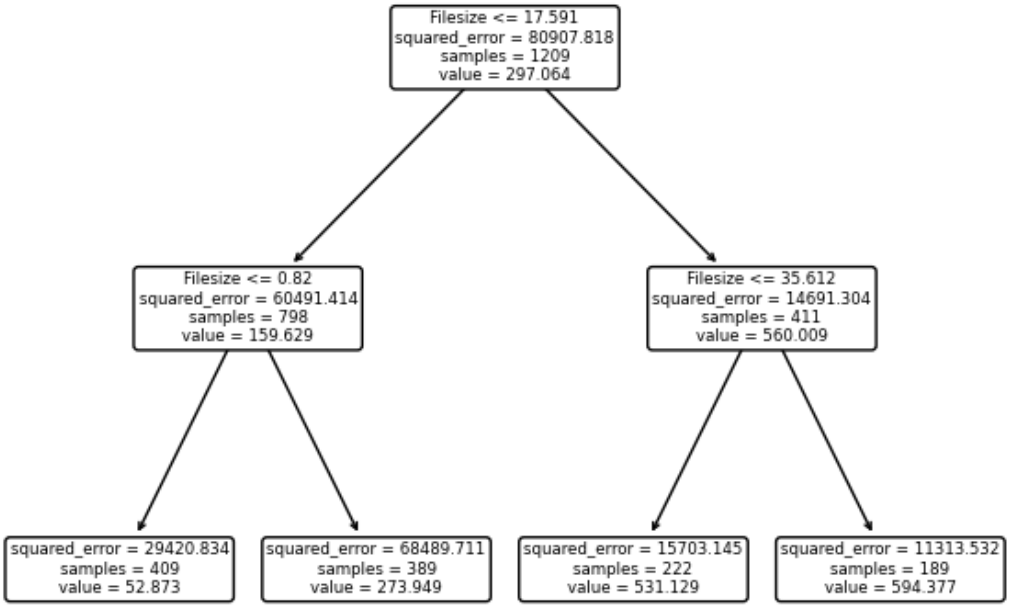

Figure 2.2: An example of a Decision Tree on the tool-resource-prediction dataset

The algorithm uses two types of randomness. On the one hand, it makes use of bagging, i.e. each decision tree selects random samples of the training dataset with replacement [16]. While a single decision tree may overfit on data, limiting its capacity for generalization to unknown data [6], using multiple decision trees with different training sets, leads to overall better generalization and reduces the variance significantly without increasing the bias [13]. The other source of randomness comes from randomly selecting a small sub-set of features for each decision tree. This de-correlates the decision trees even more, which in turn leads to better prediction of the ensemble [16]. For classification, the outcomes of the different decision trees are considered in a majority vote, while in the case of regression the mean of the trees is taken as prediction (see Figure 2.1).

2.2 Extreme Gradient Boosting

XGBoost (Extreme Gradient Boosting) is a library that provides machine learning algorithms on the basis of gradient boosting algorithms [4]. The first regression gradient boosting algorithms were introduced by Friedman [12]. The model that XGBoost uses is basically constructed out of the same building blocks as a Random Forest (see Section 2.1), i.e. the model is made up of an ensemble of decision tress. The main difference comes from how each model is trained during the learning process. XGBoost uses a concept called "boosting" where weak models are combined into a single strong model in an iterative way, which helps to reduce the bias and variance [8]. So instead of combining all the decision trees parallelly like in Random Forest, the trees are combined sequentially. The idea is that by using multiple trees after each other, the current tree corrects the error of the previous tree or in other words, each tree "boosts" the attributes that led to errors or misclassifications of the previous tree [17]. The structure of the XGBoost model can be seen in Figure 2.3.

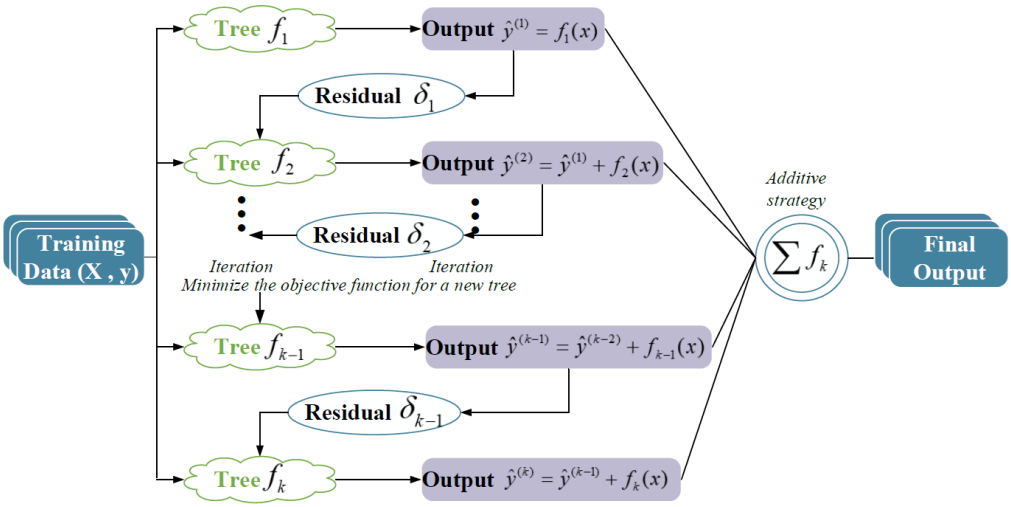

Figure 2.3: Structure of the XGBoost model (source: [11])

The output of the model is calculated with K additive functions expressed by the following equation [10]:

$$\hat{y}_i = \phi(\boldsymbol{x_i}) = \sum_{k=1}^{K} f_k(\boldsymbol{x_i}), f_k \in \mathcal{F}, \tag{2.1}$$

where $\mathcal{F}$ is the space of the decision trees, f_k represents an individual decision tree, $\boldsymbol{x_i}$ is sample i of the dataset and $\hat{y}_i$ is the output for sample i.

The model aims to minimize the following objective [10]:

$$\mathcal{L}(\phi) = \sum_i l(\hat{y}_i, y_i) + \sum_k \Omega(f_k), \tag{2.2}$$

where l is a differentiable convex loss function measuring the difference between the prediction $\hat{y}_i$ and the target y_i. Ω is a regularization term. The regularization term penalizes the complexity of the model (i.e. the complexity of a single decision tree), which leads to better generalization and less overfitting.

Since the model is trained in an additive and sequential way, following objective is minimized at the t-th iteration with the i-th instance [10]:

$$\mathcal{L}^{(t)} = \sum_{i=1}^{n} l(y_i, \hat{y_i}^{(t-1)} + f_t(\boldsymbol{x_i})) + \Omega(f_t) \tag{2.3}$$

This implies that the f_t (so the decision tree) that improves the model the most, according to equation 2.2, is added greedily [10].

3 Related works

In the past, there have been several approaches aimed at optimizing resource allocation for services. The goal is the same as in this project: avoid wasting resources caused by the assignment of too many resources and prevent service failures when too few resources are allocated. Some of these methods are presented and compared to our work in this chapter.

One similar approach was given by Schneider et al [24]. They trained machine learning models on virtual network function (VNF) data. Virtual Network Functions (VNFs) are virtualized network services that run on open computing platforms and were previously run on dedicated hardware [3]. Typical VNFs that are commonly used are virtualized routers, firewalls and network address translation (NAT) services. The majority of VNFs are run on virtual machines (VMs) [3]. Normally, a VNF is invoked using a certain quantity of resources, which is set by the VNF developer beforehand. Nevertheless, VNFs usually do not require a constant amount of resources, but rather need more or less resources depending on the traffic load. A fixed allocation of resources can lead to under-allocation or over-allocation, meaning that VNFs are not able to handle all packets, resulting in packet loss and a reduction in quality of service [24]. For this reason, under-allocation is prevented by assigning a high amount of resources to each VNF instance. This on the other hand leads to waste of resources. These procedures are similar to the way Galaxy handles its resource allocation for jobs. The models of their work were trained such that they predict the resource requirements given a certain traffic load. Likewise to our work Schneider et al. compared various machine learning algorithms against each other including Linear Regressors, Support Vector Regressors, Ensemble-based methods & Neural Networks. With their approach they were able to decrease the resource consumption up to 12 times lower compared to using standard fixed resource allocation [24].

Similar to the work by Schneider et al. [24], Nawrocki & Osypanka introduced a method that attempts to predict cloud resources [19]. By using anomaly detection methods and machine learning models to build knowledge, they were able to predict resource allocation, while taking into account various QoS (Quality of Service) constraints. With this they were able to reduce the costs ranging from 51% up to 85% (for PaaS/IaaS).

Ricart's work can also be classified under the same research area [22]. In his work, he has produced a method for resource prediction in the field of nanoelectric circuit design. By using data from previous circuit designs he was able to predict resources, such as runtime, CPU time, RAM memory, leakage and area utilization. The prediction accuracy was compared with different Machine Learning model such as Classification And Regression Trees (CART), Linear Models, Support Vector Regressors (SVR), MARS (Multivariate Adaptive Regression Splines), Neural Networks & Random Forests.

All presented works propose similar methods, namely the usage of Machine Learning models to predict computational or other forms of resources for different kinds of services. In this context, this project likewise brings forward a comparison of different Machine Learning algorithms, which aim to predict memory allocation. What makes this work stand out is the fact that it applies the methods to data from the European Galaxy server (https://usegalaxy.eu), and in doing so, examines the execution of tools in the field of DNA/RNA analysis and other areas of bioinformatics. One of the main contributions of our work to the problem of resource prediction is that it gives insights into the resource consumption of tools run on Galaxy. In addition to that, this project brings forward the possibility to give prediction intervals for new unseen data to allow investigations on the trade-off of resource costs and quality of service as described in Section 4.4.

4 Methods

This chapter explains the technical specifications of the methods used in the project. First, the Galaxy data set and the data preprocessing steps are described, followed by a description of the training, testing, and hyperparameter optimization steps. In the final section 4.4 a method to do predictions with uncertainty is brought forward.

4.1 Galaxy job run dataset

4.1.1 Description of the dataset

The Galaxy server collects extensive data on the jobs run on the platform. This data can be used and analyzed to improve the resource allocation, such that the assigned memory for each job can be optimized. The Galaxy job run dataset used for this project has been collected for the period from 31.12.2019 to 23.05.2022 on the European server of the Galaxy network. In total the dataset consists of approximately 38 million entries with about 10 GB in total size. The Galaxy job run dataset can be found here. In Table 4.1 the recorded job attributes are shown. An excerpt of the dataset can be seen in Figure 4.1.

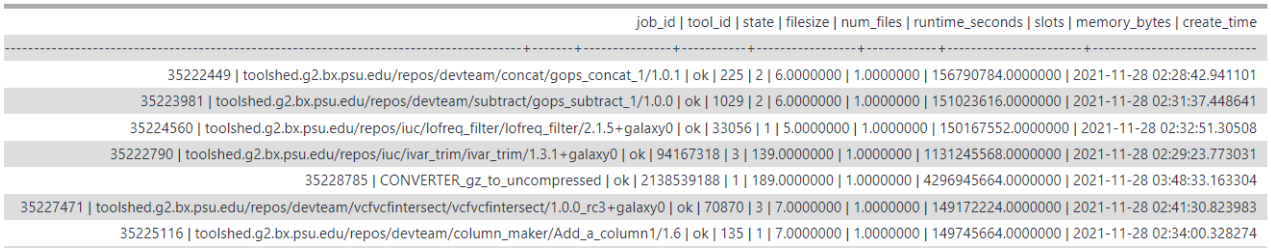

Figure 4.1: Excerpt of the Galaxy job run dataset

Attribute	Description
job_id	Unique id representing each job
tool_id	The name of the tool (with version) used for the job
state	Flag that indicated if job was run successfully
filesize	Total size of the files used for the tool in bytes
num_files	The number of files used for the job
runtime_seconds	Total runtime of the job in seconds
slots	Number of CPU cores assigned by Galaxy
memory_bytes	Maximum memory usage in bytes
create_time	Creation date and time of the job

Table 4.1: The recorded job attributes

To reduce the dataset size and make it more manageable, additional preprocessing steps have been done, which are described in the following section.

4.1.2 Preprocessing

Reducing dataset size

For our approach only a subset of the recorded attributes of the original Galaxy job run dataset are relevant. The attributes *job_id & runtime_seconds* can be removed, since they are not necessary for our case. The attribute *state* can be left out, since the query to fetch the data from the Galaxy server already only considered jobs, which were run successfully (i.e. *state* == *OK*). The remaining relevant attributes are listed in Table 4.2.

In addition to this, empty characters as well as trailing zeroes for the attributes *filesize, num_files, slots & memory_bytes* were removed, since these fields are integers and do not need decimal places. Furthermore, some entries contained no values for *filesize, num_files or memory_bytes* or had invalid combinations for *filesize & num_files* (e.g. *num_files* = 0 but *filesize* > 0) which were also removed.

These steps reduced the total size of the dataset to about 3 GB, leaving about 26 million entries (previously there were 38 million entries).

Relevant attributes
tool_id
filesize
num_files
slots
memory_bytes
create_time

Table 4.2: Relevant job attributes

Filtering faulty data

Currently the tools run on the Galaxy platform are assigned a fixed amount of memory. How much each tool is assigned is given in the Galaxy repository by the tool_destinations file (can be found here). Tools which are not configured in this file are assigned a default value of 1 GB for memory. The maximum memory is bounded to 1 TB from Galaxy. If a job fails, it is restarted with twice the amount of memory as before. Tools can get restarted up to a maximum of 3 times. This means that that the maximum memory usage (if the job gets restarted 3 times) is given by:

$$max\_memory = initial\_assigned\_memory * 2^3 = initial\_assigned\_memory * 8 \quad (4.1)$$

Using this information, the dataset was filtered for entries, which exceed memory bytes over 1 TB as well as entries, that surpass the maximum value given by Equation 4.1. This further reduced the dataset to about 2.75 GB. These removed faulty entries were collected into a separate file which can be found here. This might be useful in the future if one decides to investigate possible errors in the data recording step of Galaxy.

Regardless of whether such errors are due to any bugs in the code, server dysfunction, errors in the recording process, or a mix of any of these things, the fact that these errors exist puts the validity of the rest of the dataset in question.

Removing outliers

Through data analysis, it occurred that some tools have data points whose *memory bytes* are very far away from most other data points. Since it is not possible to find out if jobs in

the dataset are initial runs or whether they got repeated, it is reasonable to assume that these outliers might just be jobs which got repeated. Since our goal is to predict the memory of jobs in the initial run, we want to remove such data points. We do this by calculating the mean and the standard deviation of *memory bytes* and remove points that lie above the mean plus 2 times the standard deviation. To understand the influence of these outliers, experiments have been done which are discussed in Section 5.2.

4.2 Training and evaluation pipeline

This section of the report outlines several decisions related to the training and evaluation of the machine learning models. For the comparison of different methods Random Forest, XGBoost, Linear Regression and Support Vector Regression (SVR) were selected as Machine Learning models. The implementation of these models can be found in the *estimator.py* file which lies in the *src* folder of the master project GitHub repository [7].

4.2.1 Base estimators

For the base estimators of the Linear Regression and SVR all parameters were kept as their default. The same was done for Random Forest and XGB with the difference of setting the number of trees, *n_estimators*, to 200 & *random_state* to 0 for both models. The hyperparameters of all models are later optimized as described in Section 4.3 and shown in Section 5.5.

4.2.2 Training and evaluating the regressor

For the training of the regressor the features *filesize*, *num_files* and *slots* are used as input and *memory_bytes* is used as the target. The training and evaluation process in general is structured as following: A specific version of a tool is used as data and it is loaded. After this the data points are split into train and test set with a proportion of 80% and 20%. The train set is then used to fit the model using 5-fold cross-validation after which the best model is

extracted and evaluated on the test set. Cross-validation is helpful since it helps to avoid overfitting and it gives us first insights about which methods, procedures and measures work best. The performances of the models are hereby evaluated using the R2 Score.

4.3 Hyperparameter Optimization

After finding out which methods and approaches work best, Hyperparameter Optimization is applied using *HalvingGridSearchCV* with a 5-fold cross-validation [1]. The results of this optimization are described in Section 5.5. The following parameter spaces are explored during the optimization process:

Random Forest parameter space:

- n_estimators = [50, 100, 200, 500]
- max_depth = [None, 4, 16, 32]. This is used to avoid overfitting. Experiments with our data showed that most of the time the depth of the trees varies between 2 and 45, so these values are covered. With *None* the tree is expanded until all leaves are pure or until all leaves contain less than min_samples_split samples.
- min_samples_split = [2, 4, 8]. Increasing this value reduces the number of splits, therefore avoiding overfitting.
- min_samples_leaf = [2, 4, 8]. Helps to control overfitting as well.

XGB parameter space:

- learning_rate = 8 samples from log_space [0.003 to 0.3]
- n_estimators = [50, 100, 200, 500]
- max_depth = [2, 6, 16, 32, 64]. 6 is default tree depth for XGBoost. This parameter can avoid overfitting.

The Linear Regressor is not optimized since there are no tunable hyperparameters.

SVR parameter space:

- kernel = ["rbf", "sigmoid", "poly"]
- C = [0.01, 0.1, 0.5, 1, 2, 4]
- gamma = ["scale", 0.001, 0.01, 0.1, 1]

4.4 Prediction with uncertainty

As mentioned several times in this report, it can happen that jobs have to be restarted for various reasons. One possible reason is that the initially allocated memory is not sufficient for the run. If a job fails, it will be restarted with twice as much memory as before (as mentioned earlier in Section 4.1.2). One concern therefore is to investigate whether it is possible to give our algorithms the probability with which our job should succeed on the first attempt. This gives us the opportunity to trade off between optimizing resources as much as possible and the ability of a tool to succeed on the first try.

To make this understandable, here is an example: We tell our algorithm that for the execution of a tool we want the job to be successful on the first attempt with a probability of 70% in terms of the required memory. For this instance, our algorithm predicts that the job will require 10 GB of memory. In another case, we specify our algorithm that the job should be executed successfully with a higher probability e.g. with 90% on the first try. From this constraint, our algorithm in turn derives a prediction of 15 GB. This illustrates the option to trade off between a better resource allocation and the successful execution of a job.

4.4.1 Prediction intervals

The implementation of this functionality is possible for the Random Forest but not for the XGBoost model using so-called prediction intervals. A prediction interval specifies an interval in which we expect our prediction to fall with a particular probability [14]. It provides probabilistic upper and lower bounds on the estimate of our algorithm. This is useful

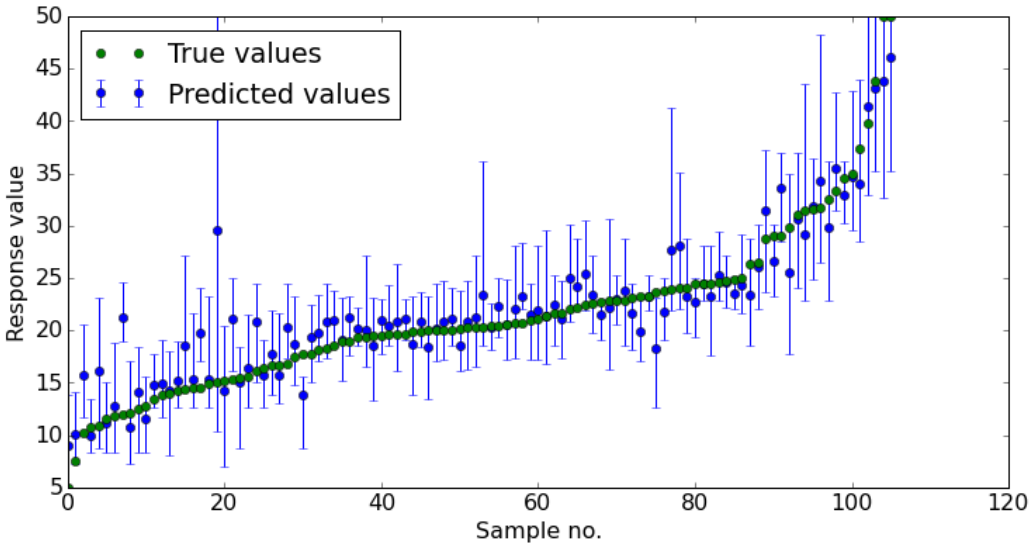

Figure 4.2: Plot of the true values and 90% prediction intervals [23]

because it is often advantageous to specify an interval with a certain degree of confidence, that contains the response value, rather than giving a single number as the predicted value. For example a 95% prediction interval for the new data point x and the prediction y is given by [18]:

$$I(x) = [Q.025(x), Q.975(x)] \tag{4.2}$$

This implies that the prediction y lies with high likelihood in the interval $I(x)$. The range of this prediction interval can differ significantly with x and depends on the data the model was trained with [18].

In Figure 4.2 you can see an example where about 90% of the samples were to lie within the prediction intervals, and in Figure 4.3 the percentage for the prediction intervals was set to 50%. In both figures, it can be observed that the prediction intervals are smaller for more accurate predictions due to the fact that the model has more confidence in the prediction at these points.

Quantile Regression Forests are one way to determine confidence intervals for Random Forests [18]. The underlying concept of Quantile Regression Forests is that rather than recording the average value of the response variable in each tree leaf in the forest, all

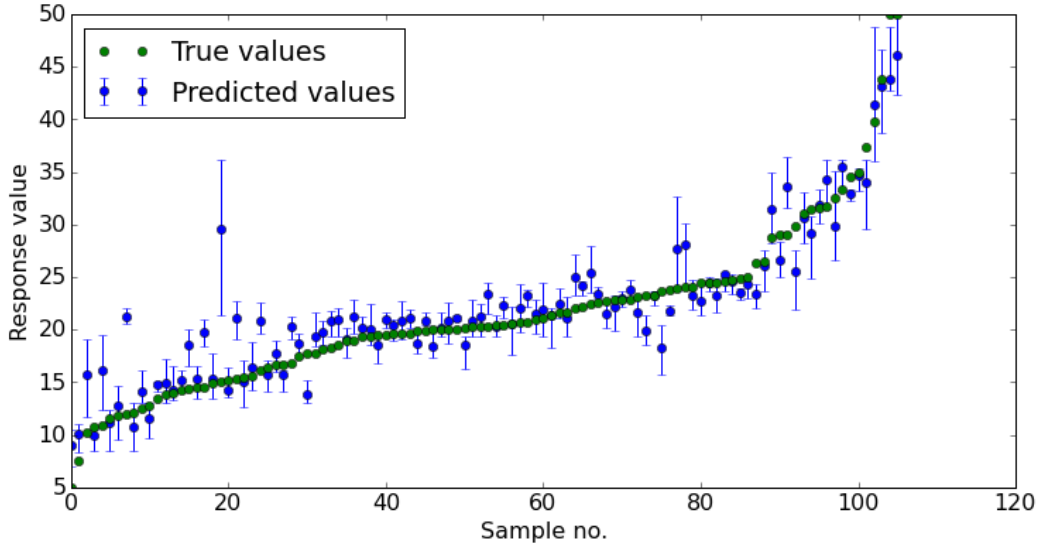

Figure 4.3: Plot of the true values and 50% prediction intervals [23]

observed responses in the leaf are recorded [23]. Thereby the full conditional distribution $P(Y <= y|X = x)$ of the response values for each x can be obtained. As an example, the 90% prediction intervals would comprise the area between the 5 and 95 percentiles of the distribution of the response variables.

To get the prediction intervals from a Random Forest, all of the individual decision trees have to be expanded fully, such that each leaf contains only one value [23]. Then, a prediction gives us the individual response variables on which the distribution is built on, if the forest is sufficiently big [23].

To use the prediction intervals with our algorithm, the following steps are performed: The user gives as input a dataset of a particular tool on which to make the prediction and a probability between [0.0, 1.0], which is used to calculate the prediction intervals. The algorithm then takes the maximum value of each prediction interval as the prediction. In theory, a job run on Galaxy with this prediction is less likely to fail due to lack of memory.

5 Results

5.1 Removing faulty data

First of all, experiments were done to judge the effects of the data pre-processing steps. In this part the removal of faulty data as described in Section 4.1.2 was inspected. To do so, models were trained and evaluated on 5 different tools. The 5 tools were selected because they had frequent faulty entries as was found during pre-processing. The models were trained using the parameters given in Section 4.2.1 and the pipeline described in Section 4.2.2. In order to allow a fair comparison, each individual dataset consists of 10000 samples. Out of these 10000 samples, 500 samples represent faulty data as defined in Section 4.1.2. In Table 5.1 the R2 scores, before and after removing faulty data, are shown for each model. As Table 5.1 shows, almost all models display an improvement across the different datasets

Dataset	Random Forest	XGB	Linear Regression	SVR
fastqc/0.72	-0.13 → 0.85	-0.17 → 0.86	0.00 → 0.82	-0.01 → 0.89
ivar_trim/1.2.2	-0.93 → 0.86	-1.50 → 0.87	0.00 → 0.77	-0.02 → 0.84
ivar_removereads/1.2.2	-0.51 → 0.64	-0.64 → 0.68	0.00 → 0.74	-0.03 → 0.70
cutadapt/1.16.5	-0.82 → 0.89	-1.64 → 0.89	0.05 → 0.13	0.05 → 0.90
mimodd_reheader/0.1.8_1	-0.37 → -0.12	-0.47 → -0.51	0.00 → 0.37	-0.02 → 0.16

Table 5.1: R2 Score of the models before and after removing faulty data

when the faulty data is removed. Although the datasets are comprised of only 5% faulty data, the improvements are quite drastic. There is only one case where the R2 score decreased, and this is for dataset *mimodd_reheader/0.1.8_1* & model *XGB*. A look at the training results shows that the mean absolute error has improved from 10.30 → 0.03 (the mean absolute errors are not given for the sake of clarity in this document). This indicates that there are a few (perhaps only one) bad predictions that are very strongly penalized by the R2 function, while the mean absolute error does not penalize this nearly as much.

5.2 Removing outliers

Another pre-processing step that needs to be examined is the removal of outliers as explained in Section 4.1.2. For this 4 of the most popular tools were selected with 10000 samples per tools. The models were trained using the parameters given in Section 4.2.1 and the pipeline described in Section 4.2.2. As can be seen in Table 5.2 especially the Random Forest and XGB models benefit from the removal of the outliers. E.g. for *rna_star/2.7.5b* the R2 Score of Random Forest improves from -0.33 to 0.04 which is quite significant. The same can be said about the XGB model. The Linear Regressor and SVR do not really benefit from the outlier removal. In some cases it even worsens the scores.

Dataset	Random Forest	XGB	Linear Regression	SVR
rna_star/2.7.5b	-0.33 → 0.04	-0.35 → 0.07	0.05 → 0.03	0.06 → 0.06
bowtie2/2.3.4.3	-0.18 → 0.07	-0.15 → 0.07	0.04 → 0.01	0.05 → 0.05
hisat2/2.1.0	-0.15 → 0.06	-0.05 → 0.07	0.10 → 0.06	0.06 → 0.05
bwa_mem/0.7.17.1	-0.21 → -0.01	-0.28 → 0.00	0.01 → -0.01	0.00 → -0.01

Table 5.2: R2 Score of the models before and after removing outliers

5.3 Correlation analysis

To get a better understanding of the underlying relations of the dataset, the Pearson correlation coefficient between *filesize* and *memory_bytes* was calculated for each tool. The results of these calculations were saved to a seperate file (which can be found here). Additionally, the number of samples per tool in the dataset was saved. This is helpful because many tools have a perfect correlation of 1.0, due to the fact that there are only few samples (often only 2).

One thing that stands out is that some of the tools (about 300 of total 4800 tools) have a moderate or even strong negative correlation. While this is nothing inherently wrong, one would assume that as the file size increases, the memory consumption would also go up, so a positive correlation should be present. As mentioned earlier in other sections, this makes the validity of the dataset put into question. Another dubious aspect is that in some cases there are major differences in the correlation between different versions of the same tool. As

Version	Pearson correlation filesize $\longleftrightarrow$ memory_bytes	nr_samples
0.4	0.99	5
2.3.4.1	0.74	130
2.3.2.2	0.53	37
2.4.2	0.31	48286
2.4.5	0.30	6031
2.3.4.3	0.25	97465
2.2.6.2	0.24	161
2.3.4.2	0.21	355
0.2	0.01	16
0.3	-0.16	3

Table 5.3: Pearson correlation for different versions of *bowtie2*

can be seen Table 5.3. Of course, this must be taken cautiously, as the number of samples is not equal for all versions to make a fair comparison.

Using the information from the calculated Pearson correlation coefficients, two types of experiments were conducted, which are described in the following sections.

5.3.1 Moderate-high correlation

In this part, we examine the ability of our models to make predictions based on data sets that show moderate to strong correlation. For this, tools with moderate correlations of 0.35 up to strong correlations of 0.95 were used, which are listed in Table 5.4. For each tool 10000 samples were taken as input and the models were trained & evaluated using 5-fold cross validation. The results of the runs can be seen in Figure 5.1.

Dataset	Pearson correlation coefficient
lofreq_indelqual/2.1.4	0.95
bamleftalign/1.3.1	0.74
fastqc/0.73	0.66
umi_tools_extract/0.5.5.1	0.55
bedtools_intersectbed/2.30.0	0.35

Table 5.4: Tools with moderate to high correlation

Figure 5.1 clearly shows that for datasets with very high correlation, all models perform quite well. For the tool *lofreq_indelqual/2.1.4* Random Forest, XGB and Linear Regression perform equally well, having a R2 Score of about 0.95 or higher. For this case the Support Vector Regressor performs the worst. This could be due to the fact that this model has more hyperparameters than the other models to choose from, which may need to be optimized.

For the tools *bamleftalign/1.3.1* and *fastqc/0.73*, which have a lower correlation, the Linear Regressor performs worse since there is no longer a clear pattern of linearity visible in the data. The other models perform all equally well with R2 Scores of about 0.75 for *bamleftalign/1.3.1* and 0.9 for *fastqc/0.73*. As for the data with even lower correlation, all models do not perform as well with an R2 score varying between 0.0 and 0.2.

Overall, we can observe a clear tendency, which is that, the greater the correlation between *filesize* and *memor_bytes*, the better all models perform. This trend can also be seen in Figure 5.2 where the model performances are plotted against the correlation of each dataset.

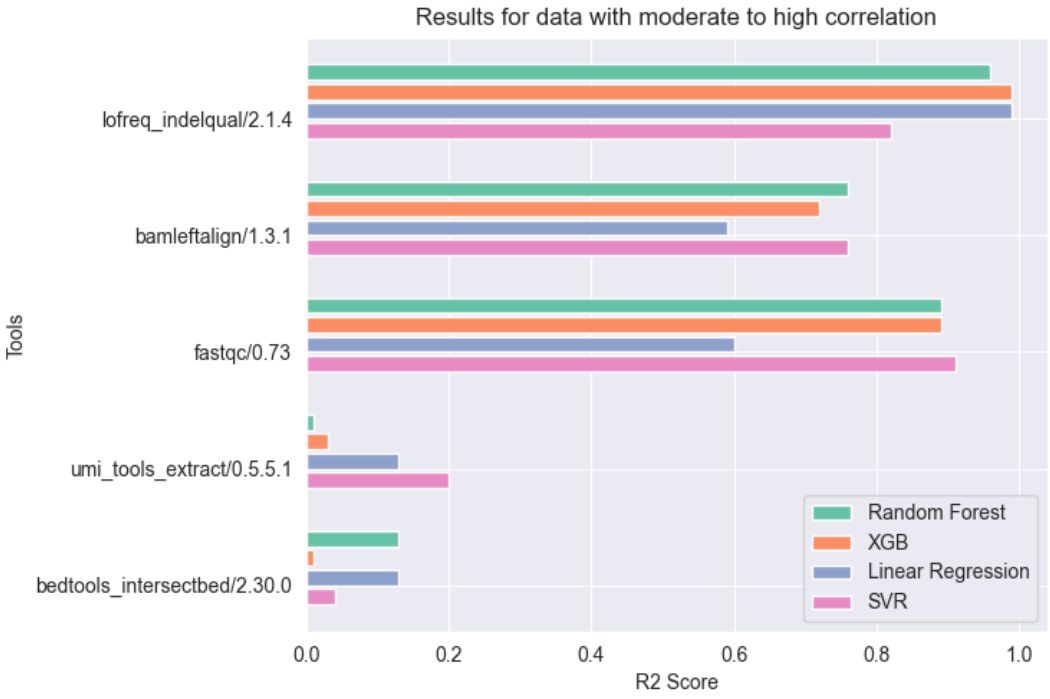

Figure 5.1: R2 Score of the models using moderate-high correlation data

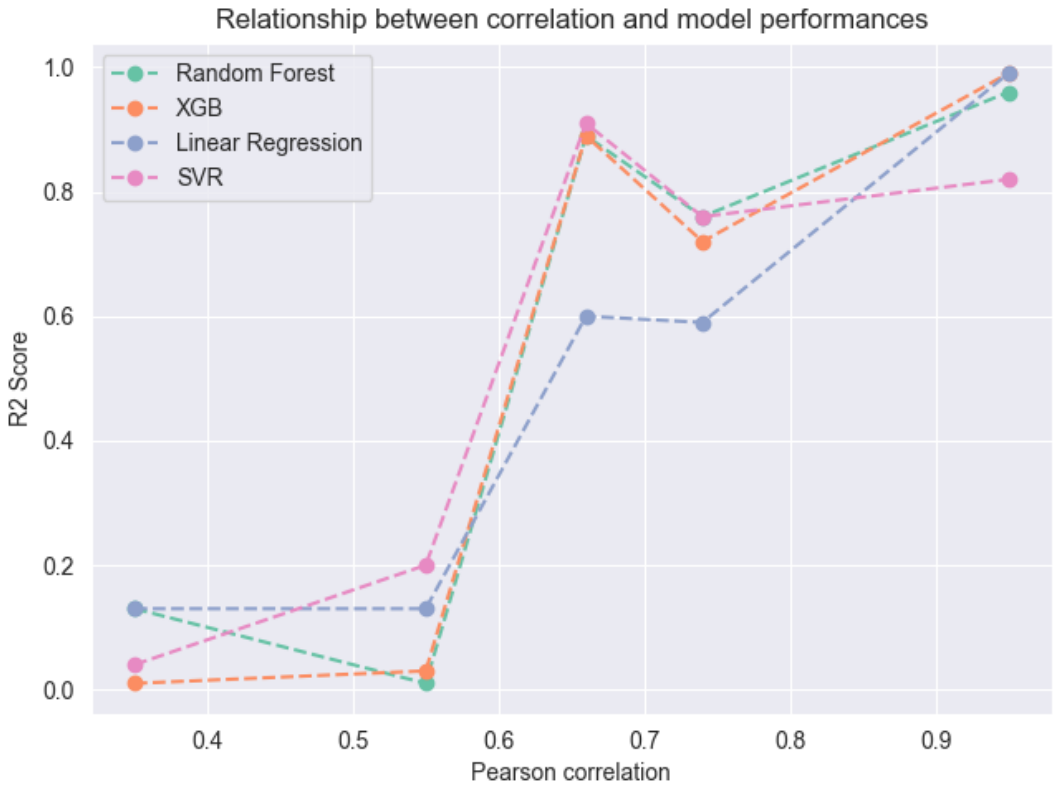

Figure 5.2: Model performance in relation to correlation for moderate-high correlation data

5.3.2 Low-moderate correlation

The same examination as in Section 5.3.1 can be done for tools which show low to moderate Pearson correlation between *filesize* and *memory bytes*. A subset of 5 tools that meet this criteria are listed in Table 5.5. Their correlation coefficients range from 0.01 up to 0.45.

Dataset	Pearson correlation coefficient
fastp/0.20.1	0.45
vcf2tsv/1.0.0_rc3	0.31
rna_star/2.7.2b	0.16
bg_diamond/2.0.8.0	0.07
samtools_idxstats/2.0.3	0.01

Table 5.5: Tools with low to moderate correlation

Using the set from Table 5.5 with 10000 samples per tool, all models have been trained applying 5-fold cross-validation, after which the best instance has been evaluated on the test set. The results of these runs can be seen in Figure 5.3.

For the dataset with the highest correlation of 0.45 *fastp/0.20.1*, all models beside the Linear Regressor perform quite well, with an equally good R2 Score of around 0.6. For the other datasets which have a correlation of 0.31 or lower, the R2 Score of all models vary greatly, with the general performance not being that good. What stands out is that the XGB model performs the worst for all datasets beside *fastp/0.20.1*, with R2 scores ranging from -0.6 to -0.15. This again might be due to the fact that the hyperparameters of XGB need to be tuned more than for the other models.

In Figure 5.4 the model performances are plotted against the correlation of the datasets. Again, a clear upward trend in the performance of the models is evident with increasing correlation of the dataset. The only dataset that stands out is the tool *bg_diamond/2.0.8.0* which has a correlation of 0.07. For this tool the Random Forest, Linear Regressor and SVR perform relatively well compared to the data points around it. This might be explained by looking at the importance the Random Forest model gives to each input feature. These are given in Table 5.6. For all datasets beside *bg_diamond/2.0.8.0*, the feature *Filesize* was given an importance of 1.0. For *bg_diamond/2.0.8.0* the importance of *Filesize* and *Number of files* is almost equally important with their corresponding values being 0.55 and 0.45. This is probably the explanation why for *bg_diamond/2.0.8.0* the models partly perform better.

Table 5.6 moreover illustrates one of the major drawbacks of the dataset: the models rely mostly on the *filesize* feature, which means when there is no greater correlation between *filesize* and *memory bytes*, the models perform bad or worse. The models work best when there is a high correlation between filesize and memory bytes as shown in Section 5.3.1. In addition to that the input feature *Slots*, which resembles the number of CPU Cores assigned by Galaxy for the job, is equal nearly in every sample in each dataset. Therefore no useful information can be extracted and accordingly the feature importance is 0.0. All in all, there are too few useful features in the dataset, so the models are too dependent on just one feature. This is even more problematic since about 50% of the tools show a correlation between *filesize* and *memory bytes* lower than 0.5, meaning that prediction for a majority of the tools is difficult.

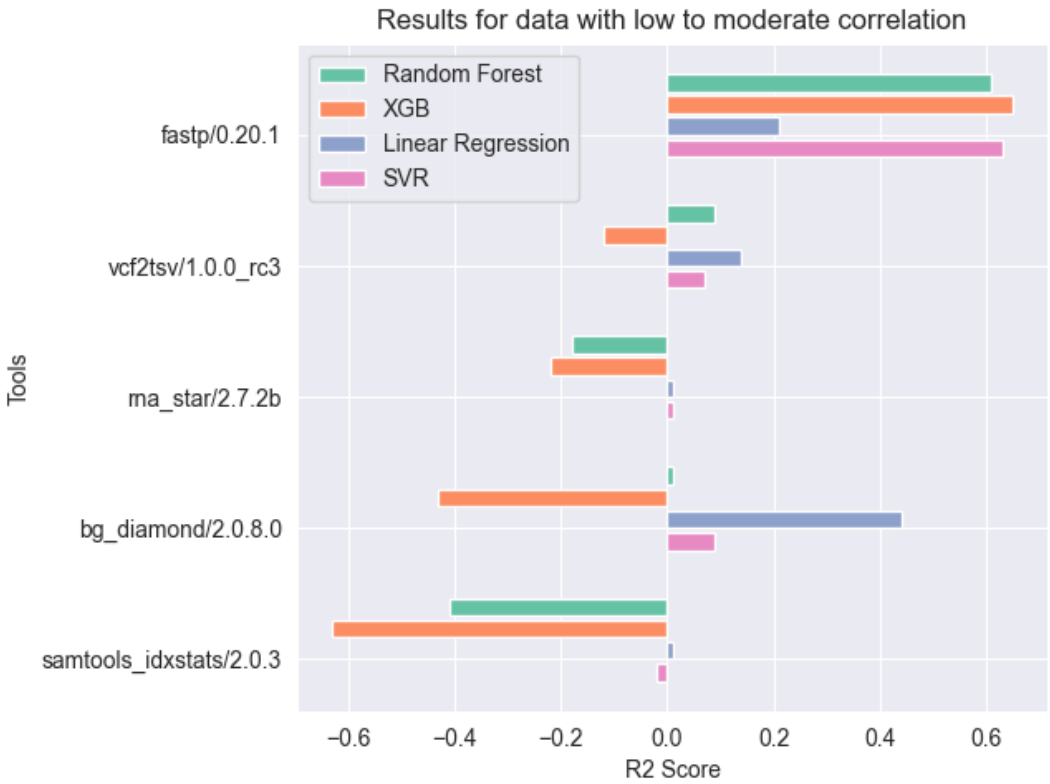

Figure 5.3: R2 Score of the models using low-moderate correlation data

	Feature importance		
Dataset	Filesize	Number of files	Slots
fastp/0.20.1	0.97	0.03	0.00
vcf2tsv/1.0.0_rc3	1.00	0.00	0.00
rna_star/2.7.2b	0.97	0.03	0.00
bg_diamond/2.0.8.0	***0.55***	***0.45***	0.00
samtools_idxstats/2.0.3	1.00	0.00	0.00

Table 5.6: The given importance of Random Forest for the input features

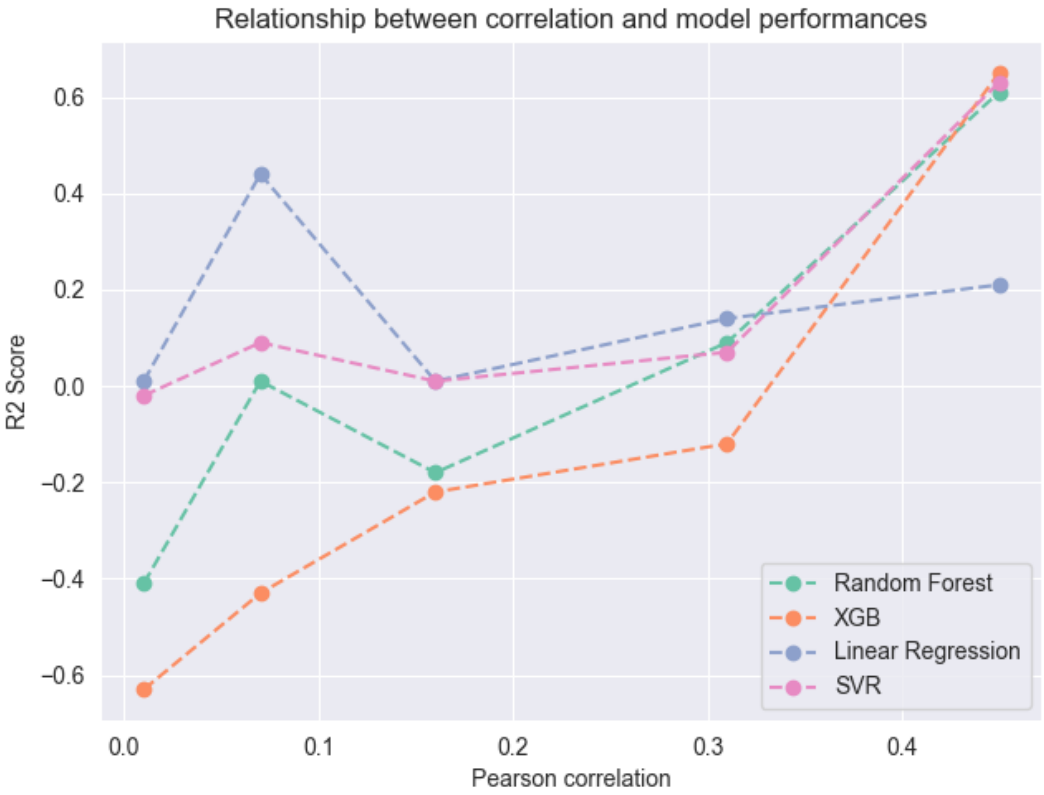

Figure 5.4: Model performance in relation to correlation for low-moderate correlation data

5.4 Performance on other datasets

In addition to the data we used from the European Galaxy instance, we also have access to data from the main Galaxy server (https://usegalaxy.org), which was provided by Kamali [15]. Unfortunately, the data is limited to a total of only 2 tools, namely bowtie2 and hisat2, where the used version for both tools is not known. After transforming the data to a format we can use, the Pearson correlation between *filesize* and *memory bytes* was calculated with the following results:

Dataset	Pearson correlation	Number samples
hisat2 (Kamali)	0.66	2797
bowtie2 (Kamali)	0.62	3963

Table 5.7: Correlation of Kamali's data

As seen in Figures 5.5 and 5.6 both datasets show some kind of logarithmic growth. However for *hisat2* there are some data points at the top of Figure 5.6 which show a strong variance in *filesize* while having the same amount of *memory*. The same pattern is visible for *bowtie2* in Figure 5.5. In addition to that, on the left side of Figure 5.6 there are data points visible which have a big variance in *Memory bytes* while having a fixed *filesize* around 0 GB. These patterns exist not only in Kamali's data but in the data we used for this project as well. As mentioned more than once, they cast doubt on the data recording process of Galaxy. How should the execution of a job with a filesize of a few kilobytes, consume 30 GB of memory, while filesizes from 10 to 20 GB consume the same amount?

Using the data from both of these tools, all models were trained and evaluated as described in Section 4.2.2. The results can be seen in Figure 5.7. The Linear Regressor performed worst out of all the models for both tools. This might be due to the non-linear shape of both datasets as can be seen in Figures 5.5 and 5.6. For *bowtie2* all models performed equally well with an R2 Score of about 0.9. Regarding the hisat2 dataset, SVR scored worse than Random Forest and XGB with an R2 Score of approximately 0.55. In contrast Random Forest and XGB had about the same score of 0.7. All in all, the models performed worse for *hisat2* than for *bowtie2*. This can be caused by multiple reasons. One is that the dataset for *hisat2* has about 30% fewer samples than *bowtie2*. Therefore, this might effect the generalization performance. Another possible reason is that, as discussed and shown in

Figure 5.6, there exist a substantial amount of data points that show a great variance for fixed *filesize* or *memory* which possibly leads to a worse score.

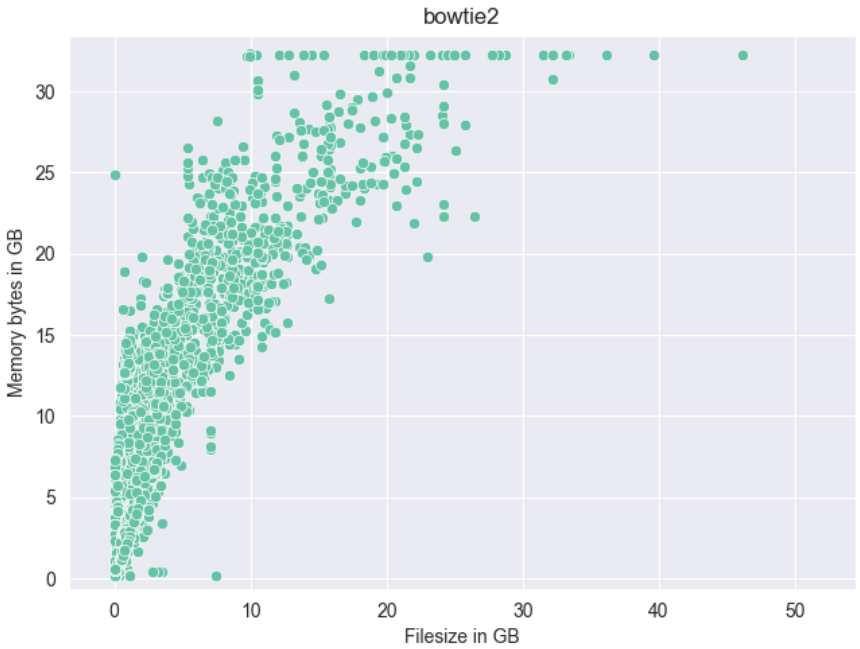

Figure 5.5: Filesize vs Memory bytes of bowtie2 (Kamali)

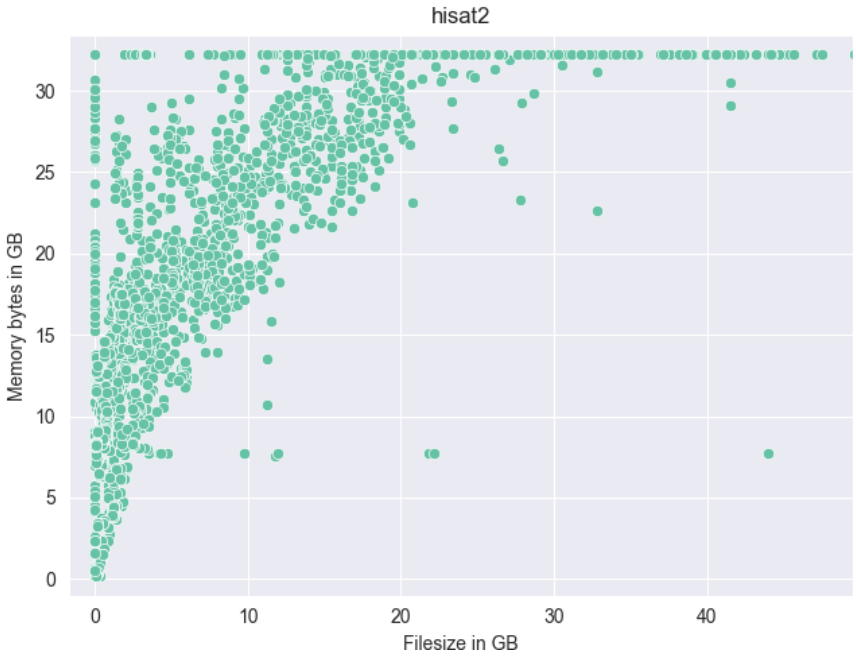

Figure 5.6: Filesize vs Memory bytes of hisat2 (Kamali)

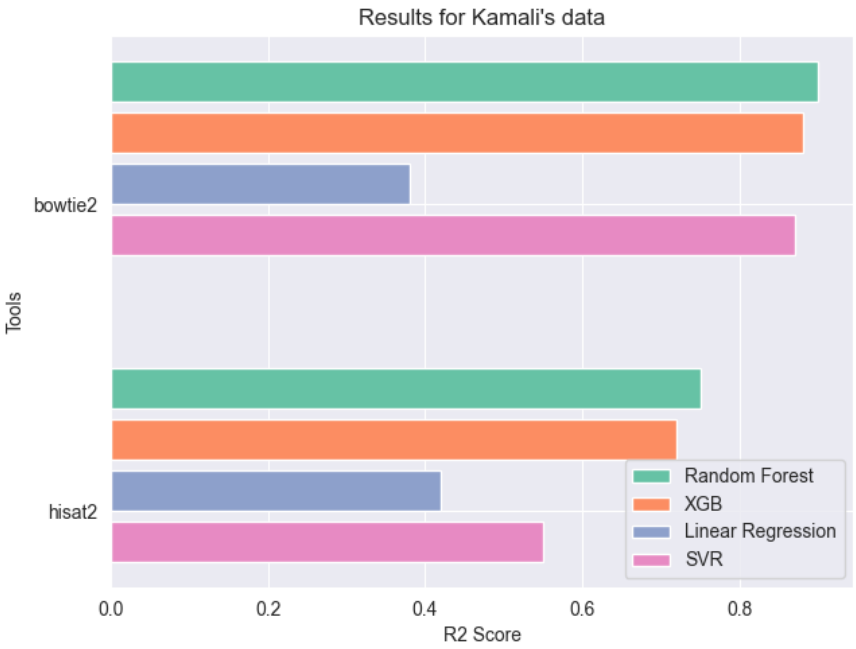

Figure 5.7: Results for Kamali's data

5.5 HPO & comparison to Galaxy baseline

In this section a comparison to Galaxy's current method of assigning fixed amounts of memory for the execution of tools is done.

To get a representative selection across all tools, 4 groups of tools were defined. For each group, two tools were selected with 10000 samples respectively. The selected tools are shown in Table 5.8 with their corresponding Pearson correlation and average memory usage.

Group	Tool	Pearson Correlation	Average Memory [GB]
High Correlation	lofreq_indelqual/2.1.4	0.95	0.21
	bamleftalign/1.3.1	0.74	0.34
Low Correlation	vcf2tsv/1.0.0_rc3	0.28	0.14
	rna_star/2.7.2b	0.20	56.72
High Memory	rna_star/2.7.5b	0.24	60.35
	kraken2/2.1.1	0.10	36.82
Low Memory	fasta2tab/1.1.1	0.29	0.20
	gmx_sim/2020.4	0.21	0.50

Table 5.8: Selected tools with their corresponding group, correlation and memory usage

To evaluate the best possible memory prediction, the models need to be optimized first. For this Hyperparameter Optimization is done as described in Section 4.3. In addition to that StandardScaler from the scikit-learn library was used for SVR and Linear Regression since both models are not scale invariant in contrast to Random Forest and XGBoost. In Table 5.9 the R2 Scores for each model & dataset is shown before and after doing Hyperparameter Optimization. For each row (dataset) the best model is highlighted.

In almost all cases across the models, there were improvements by optimizing the hyperparameters. For Random Forest and XGB the improvements were very significant. E.g. Random Forest had an R2 Score of -0.33 for *rna_star/2.7.5b* before and a score of 0.09 after optimization. The XGB model had about the same improvement for *rna_star/2.7.5b*. As expected all models perform quite well on *lofreq_indelqual/2.1.4* since it has a strong correlation of 0.95 between *filesize* and *memory bytes*. For all other datasets Random Forest was the model with the best score, beside for tool *fasta2tab/1.1.1* where SVR performed best. However, there was often not much of a difference between the Random Forest and XGB scores. For the SVR model the optimization has not improved the scores as much

as hoped. Often the score got slightly worse, which may be caused by the successive halving technique used in the optimization process. In general the tools for which all models performed the best were *lofreq_indelqual/2.1.4*, *bamleftalign/1.3.1* and *fasta2tab/1.1.1*. The first two are plausible since they have a strong correlation. The tool *fasta2tab/1.1.1* on the other hand has a low correlation of 0.29. The good results for this tool can be explained by looking at Figure 5.8 where, beside a few outliers, a clear pattern of memory usage can be seen with increasing filesize.

Dataset	Random Forest	XGB	Linear Regression	SVR
lofreq_indelqual/2.1.4	0.96 → 0.98	0.99 → 0.96	0.99	0.74 → 0.86
bamleftalign/1.3.1	0.76 → 0.79	0.72 → 0.78	0.59	0.77 → 0.77
vcf2tsv/1.0.0_rc3	0.09 → 0.15	-0.12 → 0.07	0.14	-0.01 → -0.04
rna_star/2.7.2b	-0.18 → 0.04	-0.22 → 0.04	0.01	-0.01 → 0.01
rna_star/2.7.5b	-0.33 → 0.09	-0.35 → 0.09	0.05	0.07 → 0.07
kraken2/2.1.1	-0.09 → 0.18	-0.02 → 0.17	0.08	-0.01 → -0.04
fasta2tab/1.1.1	0.69 → 0.80	0.72 → 0.80	0.25	0.81 → 0.78
gmx_sim/2020.4	-0.01 → 0.10	0.01 → 0.07	0.07	0.05 → 0.06

Table 5.9: R2 Scores of the models before and after HPO

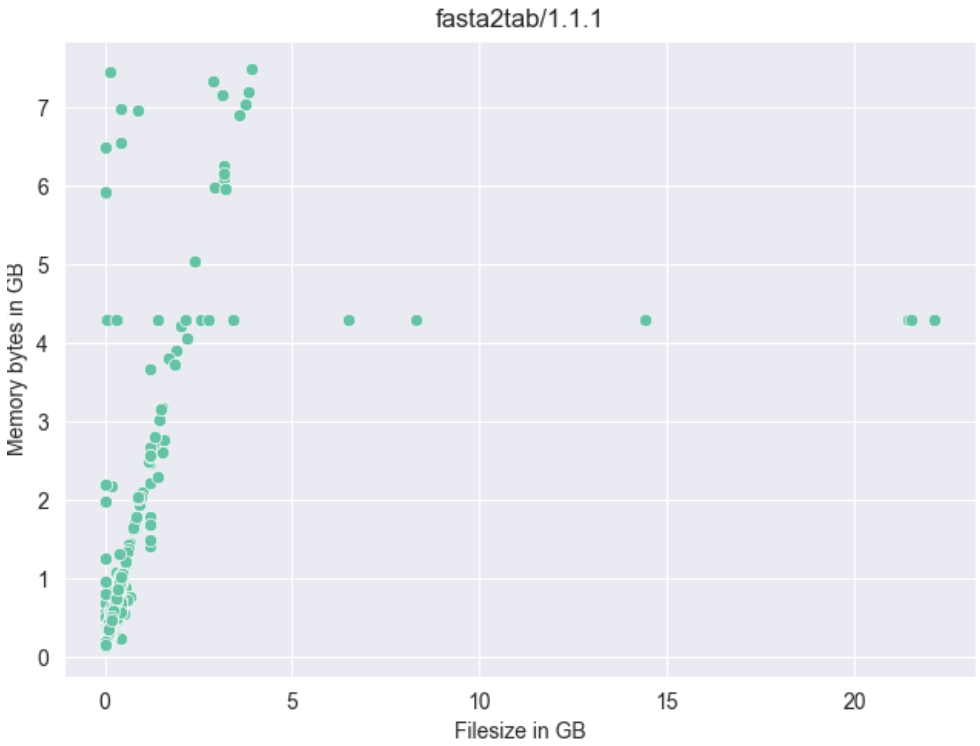

Figure 5.8: Filesize vs Memory of fasta2tab/1.1.1

5.5.1 Analysis on resource consumption

As already described in Section 4.1.2 Galaxy currently assigns each tool a fixed amount of memory. This is pre-configured in the the tool_destinations file (can be found here). Tools which are not configured in this file are assigned a default value of 1 GB for memory. Using this information and the trained models, evaluations can be done to estimate how many resources can be saved by using the trained Machine Learning models instead of the pre-assigned memory by Galaxy. For reference the tool_destinations file of the project repository was used (repository link).

Using the optimized models, the tools *kraken2/2.1.1* and *rna_star/2.7.5b* were inspected, since they have a high memory usage on average as can be taken from Table 5.8. As for both tools the Random Forest model was the best, it was chosen for analysis. The results of the analysis on the test set of both tools can be seen in Table 5.10. For *rna_star/2.7.5b* the results of the Random Forest are quite good. While Galaxy overallocates about 42 GB of memory on average, Random Forest assigns only about 14 GB too much (that is a decrease of about 65%). One drawback is that with the Random Forest model the percentage of failed jobs amounts to 23% compared to 12.25% from Galaxy. For *kraken2/2.1.1* Galaxy overallocates 41 GB whereas the Random Forest model overassigns only about 20 GB (a decrease of about 50%). Nevertheless the number of failed jobs increase for the Random Forest up to 44.95% compared to 25.25% from Galaxy.

		Average overallocation		**Failed jobs**	
Tool	**Assigned by Galaxy**	***Galaxy***	***RF Model***	***Galaxy***	***RF Model***
rna_star/2.7.5b	90 GB	42.52 GB	14.59 GB	12.25%	23.10%
kraken2/2.1.1	64 GB	41.38 GB	20.90 GB	25.25%	44.95%

Table 5.10: Comparison of resource allocation and failed jobs for Galaxy and Random Forest

5.6 Accuracy-Failure trade-off

As seen in Section 5.5.1, even though our Random Forest model was able to optimize the resource consumption compared to Galaxy, the percentage of failed jobs increased. To investigate the trade-off between accuracy and possible job failure we use the optimized Random Forest and the method described in Section 4.4. Using the same tools as before

and by providing a probability of 99% certainty to our tool, we get the results given in Table 5.11. For both tools the average overallocation decreased. In the case of *rna_star/2.7.5b* it went up from 14.59 GB to 28.33 GB and for *kraken2/2.1.1* from 20.90 GB to 28.68 GB. This behaviour is expected since the model uses the upper bound of the prediction interval, which results in a higher estimation memory-wise. It can be observed that for both tools the percentage of failed jobs decreased significantly. For *rna_star/2.7.5b* it went down from 23.10% to 13.55% achieving a similar rate as Galaxy while having much less overallocation. At the same time for *kraken2/2.1.1* it went down from 44.95% to 35.3%. This shows the effect of the prediction with uncertainty. By setting a prediction interval with the given probability, the model is able to provide a prediction that results in a more likely job success on the first try.

	Average overallocation		**Failed jobs**	
Tool	***Galaxy***	***RF Model***	***Galaxy***	***RF Model***
rna_star/2.7.5b	42.52 GB	14.59 GB → 28.33 GB	12.25%	23.10% → 13.55%
kraken2/2.1.1	41.38 GB	20.90 GB → 28.68 GB	25.25%	44.95% → 35.3%

Table 5.11: Comparison of resource allocation and failed jobs for Galaxy and Random Forest with certainty probability 99%

6 Discussion and Conclusion

For this project the Galaxy job run dataset was analyzed and different Machine Learning methods were used to predict the memory usage of future jobs. In this context, several preprocessing methods were brought forward, including the filtering of invalid data, removal of outliers and general text processing steps to reduce the dataset size. By doing so, the Galaxy job run dataset could be reduced from 10 GB to about 2.8 GB, resulting in a decrease of approximately 70%. The findings of invalid entries in the dataset and other characteristics that were discussed in this report, make us doubt the validity of the recorded dataset. Another aspect is that it is not possible to find out if jobs in the dataset are initial runs or whether they got repeated. If it is possible, Galaxy should track this because then this can be filtered since the goal is to predict the memory of the initial run.

The effects of filtering invalid data were examined and it was shown that all models benefit from the filtering of faulty data, resulting in significant improvements of the R2 score. Similarly, the removal of outliers was evaluated, which improved the results for Random Forest and XGB models as well.

Furthermore, it was shown that there is a relationship between the performance of the models and the correlation of the data between *filesize* and *memory bytes*. In general, it was apparent that a stronger correlation of the two features resulted in a more accurate and robust prediction. Equally, it became evident that for tools with low correlation, the models performed worse on average. This made one of the major drawbacks of the dataset visible: the models rely mainly on one feature, namely filesize. This means, if there is no significant correlation between *filesize* and *memory bytes*, the models perform poorly or worse. Performance is best when there is a high correlation. In addition, the input feature *slots*, which corresponds to the number of CPU cores allocated by Galaxy for the job, is almost the same in each dataset. Therefore, no useful information can be extracted. All in all, there are too few useful features in the dataset, so the models depend too much on a

single feature. This is even more problematic since approximately 50% of the tools have a correlation less than 0.5 between *filesize* and *memory bytes*, meaning that prediction is difficult for many tools.

At the end, the models were optimized using Hyperparameter Optimization and a comparison to Galaxy's method of assigning fixed amounts of memory for tools was done. It was demonstrated that by using the prediction of our models, the overallocation of memory in some cases could be reduced by 50% to 65%. This illustrates the potential usage of such Machine Learning models in the Galaxy system to optimize resource allocation and reduce wastage. While the predictions of the models led to a higher failure rate of the jobs, a method was brought forward which uses prediction intervals to generate predictions to reduce job failure rates.

This brings us to the future work that could be done using the findings of this project. It would be of great interest to see how the proposed machine learning models would perform in a real scenario in the Galaxy framework. One could investigate how it affects the memory consumption and memory waste during the execution of tools and whether this would lead to an optimization of resources. At the same time, it would be useful to look into the job failure rates of a real scenario and see how the models perform. Another research opportunity would be to examine if, instead of training one model for each tool at a time, an entire model can be generated for multiple tools. Then the performance of this model could be compared to the models brought forward in this project.

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