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REGRESSION METHODS FOR SURROGATE MODELING OF A REAL PRODUCTION SYSTEM APPROXIMATING THE INFLUENCE ON INVENTORY AND TARDINESS

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ABSTRACT

Simulation optimization is often conducted by applying optimization heuristics (e.g., genetic algorithms) whereby the simulation model delivers the objective function value for the respective parameter set. For real world simulation models, their evaluation time is a crucial constraint. This holds especially for material requirements planning (MRP) parameter optimization of real production systems with many products, because of an extensive search space. Approximating the objective function values by surrogate models can be applied to reduce the search space. Based on a real world production system simulation model, the performance of different regression models to identify simple surrogate models for fast objective function approximation is evaluated in this paper. Specifically, a focus is put on the relationship between the MRP parameters: lot-size and planned lead time, and the performance indicators: inventory and tardiness costs. The paper evaluates a set of simple regression models and compares their objective function fit.

1 INTRODUCTION

Simulation is a valuable tool to represent the behavior of real production systems since analytical models are usually not capable of including the complex relationships and interaction between materials, production orders and resources. Specifically, production planning can be focused with such simulation models to improve and/or optimize the planning parameters (Peirleitner et al. 2017; Felberbauer and Altendorfer 2014; Altendorfer et al. 2014). However, simulation run times of real size simulation models are rather high and, therefore, most studies reduce the search space, for example, by clustering the planning parameters and evaluating only one parameter for this cluster. In Peirleitner et al. (2017), where a real production system is evaluated, e.g., only one factor is implemented for the MRP parameter lot-size, one factor for the planned lead time and the safety stock. Even though this simplification leads to an optimization search space which can be fully enumerated (within an appropriate range), a lot of improvement potential is lost by such approaches. For simulation-based optimization of each single parameter, search heuristics, e.g., genetic algorithms, can be applied to find good (optimized) solutions (see Beham et al. 2012), whereby such approaches need a larger amount of single simulation runs to perform well. In such search heuristics, each single simulation run delivers an objective value to the heuristic which defines the next parameter set, or the next generation of parameter sets, to be evaluated. Related to the high run time of real production system simulation models covering the production planning parameter effects, the applicability of such search heuristics is limited. Therefore, a more recent research stream on applying surrogate models has to be evaluated in the context of production system simulation models. In this extended simulation-based optimization approach with surrogate models, not all parameter sets are evaluated with actual simulation runs. A surrogate model is created from the actually observed interdependencies between the parameters and

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the simulation's response. Only promising solution points, according to the surrogate model, are evaluated with actual simulation runs. The solution quality improvement with surrogate models is related to the fit of the surrogate models to the simulation results, however generalization capabilities are also important. The surrogate assisted optimization approach requires that the response of unseen configurations can be estimated well. One approach is to use simple regression models (e.g., linear regression) to avoid an overfit of the surrogate to the observed data. However, production system literature shows that the relationship between the planning parameters lot-size and the key figures inventory and tardiness, as well as between planned lead time and these key figures are not linear (Karmarkar 1987; Altendorfer 2015; Altendorfer and Minner 2015). Therefore, simple linear regression models are conjectured to not work well. The objective of the paper is to identify simple (non-linear) regression methods, which are on the one hand generic, but provide on the other hand a good fit for the production system. This is conducted by using a real world simulation model from a previous company project. Note that data is anonymized in this paper.

The paper is structured as follows. In Section 2, some relevant literature on simulation-based optimization of production planning parameters and surrogate model applications is provided. The real world production system which is simulated is introduced in Section 3 and Section 4 provides an overview of the applied regression methods for surrogate models. The numerical results are discussed in Section 5 and some conclusions are provided in Section 6.

2 LITERATURE REVIEW

In this section, relevant literature on simulation-based optimization for production planning and surrogate-models is presented.

2.1 Simulation-based Optimization of Production Planning using Solution Heuristics

The field of simulation-based optimization (Law and Kelton 2007; Fu et al. 2005) is still a rather young research area. The efficient utilization of distributed computing infrastructures can certainly be seen as a key enabling technology allowing optimization of more complex real-world simulation models. So far, metaheuristic optimization approaches have been applied successfully in solving combinatorial optimization tasks, such as vehicle routing, production scheduling, and layout optimization (Affenzeller et al. 2015). However, with traditional mathematical methods, it is not possible to depict the complexity and the dynamics of a holistic modeled production planning process of an organization. One possibility of decision support within such complex and dynamic planning problems is the application of simulation (Negahban and Smith 2014). With simulation, production processes can be presented realistically. It is possible to show correlations between time- and capacity-dependent parameters and stochastic influences on the whole planning system (Mourtzis et al. 2014). As a consequence, various optimization results can be evaluated concerning defined quality parameters (Affenzeller et al. 2015). Recent applications of simulation-based optimization or improvement of planning parameters are Gansterer et al. (2014) who study a simulation-based optimization of MRP parameters, Jodlbauer and Huber (2008) who explore robustness and stability of production planning parameters in the field of various production planning and control systems, such as MRP. Furthermore, Hübl et al. (2013) examine the influence of dispatching rules on the average production lead time for one- or multi-stage production systems and Altendorfer et al. (2016) evaluate the hierarchical planning process with simulation. Also complex dispatching rules may be improved by using genetic programming and evaluating the generated optimization results by simulation (Beham et al. 2010; Pitzer et al. 2011; Hunt et al. 2014).

2.2 Surrogate Models for Solution Time Reduction

When applying simulation-based optimization, the evaluation of possible solution candidates is quite expensive. A single simulation run can take from multiple minutes up to hours or even days (Koziel and Leifsson 2013). When such complex problems have to be optimized, employing conventional heuristic approaches that need to execute hundreds of thousands of evaluations is not feasible due to time constraints. This is where surrogate modeling comes into play. Surrogate models are approximations to other models and can be evaluated in a much shorter time frame (Forrester and Keane 2009; Queipo et al. 2005). Given an input vector x, they yield an output value y, depending on which target is modeled. Many different surrogate modeling techniques are available in literature, e.g., linear regression (Neter et al. 1996), non-linear regression, random forests (Breiman 2001), support vector machines, gradient boosted trees (Friedman 2001), M5' trees (Quinlan 1992; Wang and Witten 1996), or Gaussian processes (Rasmussen 2004). An extensive review on Kriging (i.e., Gaussian process) surrogates for simulations has been conducted by Kleijnen (2009). Surrogate models are usually trained using a set of already known inputs and corresponding outputs, commonly referred to as dataset. When such datasets are not available yet, some simulation runs have to be executed in order to start the surrogate model building process. Once a sufficient number of simulations with different input parameters have been executed, a dataset can be built and used for model building. Usually, such datasets are split into at least two partitions. One is called the training partition, the other one is called test partition. The training partition is used to learn the actual surrogate (i.e., regression) model. Once training is complete, the test partition is used to evaluate the model's performance on unseen data, i.e., which wasn't available for training. A third partition, referred to as validation partition may be used in selecting the resulting model. Good models will only behave marginally weaker on the test partition compared to the training partition. If the model performs significantly weaker, the model building process may be subject to overfitting, i.e., the model memorized the training data, but does not generalize well and therefore cannot predict data it has not seen before good enough. This condition is undesirable (Hawkins 2004).

3 SIMULATED PRODUCTION SYSTEM

The simulation model applied for generating the dataset to train and test the regression models for their applicability as surrogate model for production planning parameter optimization is a real world model. The company for which the model has initially been built is an automotive supplier which produces transmission system components. Production planning is conducted using MRP based on a customer demand forecast that is updated regularly. The simulation model has been created within a practical optimization project to improve the production planning of this company, however, a simple enumeration scheme as also introduced in Section 1 has been applied there. In the initial study a total of approximately 57,000 simulation runs were made, using 40 replications per iteration. Some production system features are introduced in this section to better understand the planning complexity as well as the objective function results discussed in further sections.

The company supplies mechanical processed parts to different assembly lines of an internal customer on a daily basis, i.e., each day a delivery is performed to the customer. The company uses the well-known ERP (Enterprise Resource Planning) system SAP which has an MRP algorithm implemented to create production orders. Based on the stocking policy of this company no safety stock is kept and, therefore, the MRP parameters to be optimized are lot-size and planned lead time for each material (see also Hopp and Spearman 2011 for MRP). The production system produces in its original setting 116 end items, i.e., products to be sold. Based on an ABC cluster analysis, 37 end items have been identified that make up to 80 % of the capacity demand and only these items are simulated in detail. For the remaining items only the capacity consumption is simulated. 30 of the 37 end items have a sequential BOM (bill of material) structure, i.e., one raw material is processed in several mechanical processing steps until the end item is generated. For the remaining end items, which consume some semi-finished materials, 16 such semi-finished items are included in the simulation study as well. This leads to 106 planning parameters to be optimized (53 lot-sizes and 53 planned lead time values). The production system consists of 32 machines that are simulated and perform for example milling, turning and grinding operations. Most processing steps can be performed only on one machine, however, for some processing steps alternative machines exist. The dispatching of production orders is performed according to the EDD (earliest production order due date) rule and alternative machines are used to balance the order queues of the respective machines. Additionally, most materials have also one or more external processing steps, e.g., hardening and laser welding, which are simulated by an external lead time distribution. The model is created using a generic simulation framework SimGen which has been introduced in Felberbauer et al. (2012) and Altendorfer et al. (2013). The performance criterion applied in this study is the sum of inventory and tardiness costs which are reported in Section 5.

4 REGRESSION MODELS

As stated above, the regression models applied for surrogate modeling should on the one hand be simple and on the other hand provide a good fit between the simulation results and the approximated objective value. In this section, firstly the simple linear regression model is briefly introduced, which only provides the baseline for improvement by the non-linear models presented later on.

4.1 Linear Regression

In multiple linear regression models, the objective function is only approximated by linear influences of the parameters applying different weights for each parameter. The term multiple indicates that more than one parameter influence is used. Equation (1) and Figure 1 show how the objective function is approximated with such a multiple linear regression whereby ϕ is the approximated objective function, the β-values are the respective weights and the X-values are the planning parameters (Neter et al. 1996).

$$\phi = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{106} X_{106} \tag{1}$$

Since the relationship between the planning parameters and the logistical key figures inventory and tardiness costs, which add up to the overall objective value, is not linear (see also introduction section), this multiple linear regression is only applied as baseline for comparison.

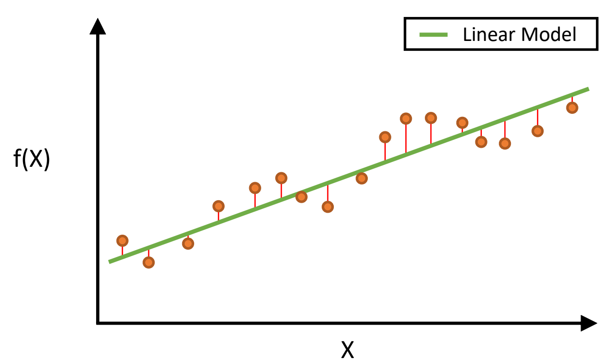

Figure 1: A linear model for a one-dimensional function.

4.2 Random Trees and Forests

Non-linear approaches include the use of so called decision trees. Given some already observed input and corresponding output variables, a decision tree can be created (Quinlan 1986). Training data is split in different dimensions according to certain criteria, e.g., to create homogenous sets of data points. Each split will then correspond to a node in the decision tree.

An exemplary decision tree with three splits is shown in Figure 2. Since it is a one-dimensional function, only one dimension (X) can be used for splitting. In this example, the first cut is done at $X < \alpha$ and two more at $X < \beta$ and $X < \gamma$. If $X < \alpha$ and $X < \beta$ are met, the left-most path in the tree will be taken and the value ϕ_1 will be predicted. If $X \geq \alpha$ and $X < \gamma$, the decision tree will predict ϕ_3. Terminal nodes, i.e., the leafs of the tree, represent the predicted values. The calculation of these predicted values also depends on the specific implementation of the decision tree, e.g., the average of all observed values in the split partition, as shown in Figure 2, can be used as prediction.

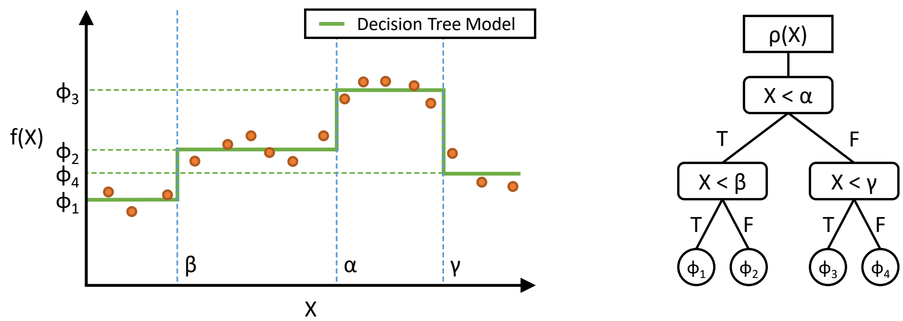

Figure 2: A decision tree model, splitting X at α, β and γ.

A random forest (Breiman 2001) is then an ensemble of such decision trees that are used to predict target variables. The number of trees is a parameter that can be configured. Each decision tree is created using a certain percentage of the available training data. Furthermore, the amount of available features for each tree during its creation is configurable. The resulting decision trees form the random forest, as depicted in Figure 3. A prediction is calculated by averaging over all predictions from the individual trees.

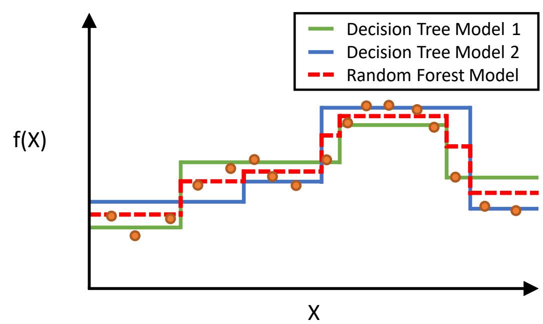

Figure 3: Two decision tree models forming a random forest model.

4.3 Regression Tree

A regression tree is a more specialized form of a decision tree. The regression algorithm first starts by constructing a decision tree, where every leaf predicts values using its own regression model, e.g., a linear regression. Once the initial tree has been created, it is checked whether or not pruning of nodes increases the model accuracy. This is done bottom-up by starting at the lowest splits. A split is temporarily removed and replaced by a new regression model, e.g., a linear regression. The algorithm then decides whether or not the previously removed split was better than the new single leaf node that uses the regression model. Therefore, the regression tree's accuracy, as well as the number of input variables required for the node before and after the replacement, are analyzed. If the split was better, it is kept, otherwise, the split is replaced by the leaf node with the new regression model, which effectively leads to the pruning of the tree, as shown in Figure 4. Usually, the decision tree is initially created with leafs that represent linear regressions for the split partitions. When pruning is started, new leaf nodes can be constructed using e.g., Gaussian process models instead of linear regression models. The maximum number of initial leafs that can initially be created depends on the chosen regression method. When employing linear regression, the maximum number l can be calculated as shown in Equation (2)

$$l = \left\lfloor \frac{d}{f+1} \right\rfloor \tag{2}$$

where d equals the number of points in the dataset and f the number of features, because each linear regression needs at least $f+1$ points for prediction and one data point can only be present in one partition. By pruning subtrees, the overall decision tree should be simplified, but model accuracy should be increased. Examples for regression trees are for instance CART (Lawrence and Wright 2001) or M5' (Quinlan 1992; Wang and Witten 1996).

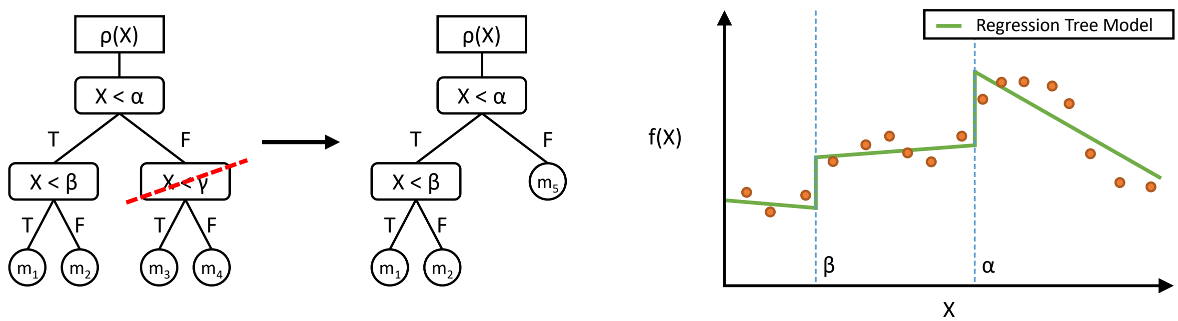

Figure 4: A regression tree model where one subtree has been pruned.

4.4 Gradient Boosted Trees

Gradient boosted trees (GBT) (Friedman 2001) are similar to random or regression trees, but do not aim to predict the dependent variable with each tree again. Instead, an initial guess may be made, for instance in form of a constant model and subsequent trees predict the residual error remaining. Thus, the sum and not the average of the prediction of all trees creates a prediction of the target variable. Still, each tree may only use a randomly chosen subset of the data and randomly chosen subset of the features. A well-known example of GBT is AdaBoost (Schapire and Freund 2012).

5 NUMERICAL RESULTS

In this work we applied the 4 regression methods: linear regression (LR), random forest (RF), regression tree (RT) and gradient boosted trees (GBT). Their performance as surrogate models for predicting inventory costs (IC) and tardiness costs (TC) of a real-world production system with respect to the dispatching parameters planned lead time and lot-size for each of the 53 materials (see Section 3) is evaluated. To generate an appropriate data sample for this numerical study, the simulation model is evaluated at 3,000 randomly chosen configurations whereby the average cost estimation from 10 replications is calculated. Thus, a total of 30,000 simulation runs have been performed and the number of evaluated combinations is based on prior experiences.

In Table 1 and Table 2 we state the coefficient of determination (R^2), mean absolute error (MAE) and mean relative error (MRE) when using only one type of planning parameter for both of the predicted costs, i.e., costs are approximated only applying the lot-size or the planned lead time parameters.

As we can observe, the models are not able to predict the costs well and some models, RF and GBT, show much better performance on the training set than on the test set suggesting that overfitting might be the problem. Specifically the R^2 values indicate a bad surrogate model fit in the test sample, whereby

Table 1: Model accuracies using lot-sizes only.

		INVENTORY COSTS (IC)			TARDINESS COSTS (TC)		
		R^2	**MAE**	**MRE**	**R^2**	**MAE**	**MRE**
LR	**training**	0.4288	926.02	0.0596	0.4191	16,648.39	0.5876
	test	0.4090	1,005.23	0.0649	0.3916	17,685.17	0.6085
RF	**training**	0.7593	655.81	0.0421	0.7588	11,329.47	0.3875
	test	0.4173	988.04	0.0635	0.4114	16,945.52	0.5626
RT	**training**	0.4288	926.02	0.0596	0.4191	16,648.39	0.5876
	test	0.4090	1,005.23	0.0649	0.3916	17,685.17	0.6085
GBT	**training**	0.7972	589.79	0.0380	0.7949	10,648.49	0.3733
	test	0.3887	1,007.21	0.0649	0.3622	17,896.34	0.6059

Table 2: Model accuracies using planned lead times only.

		INVENTORY COSTS (IC)			TARDINESS COSTS (TC)		
		R^2	**MAE**	**MRE**	**R^2**	**MAE**	**MRE**
LR	**training**	0.2625	1,036.64	0.0673	0.2863	18,854.17	0.9415
	test	0.2670	1,098.39	0.0713	0.2618	19,456.98	0.9312
RF	**training**	0.7788	764.17	0.0497	0.7361	13,541.45	0.6908
	test	0.2330	1,143.45	0.0743	0.2630	19,507.13	0.9365
RT	**training**	0.2625	1,036.64	0.0673	0.2863	18,854.17	0.9415
	test	0.2670	1,098.39	0.0713	0.2618	19,456.98	0.9312
GBT	**training**	0.7754	650.34	0.0423	0.7786	11,804.17	0.5813
	test	0.2319	1,116.46	0.0727	0.2324	19,933.61	0.9471

the slightly higher R^2 values for lot-size indicate a higher influence of this parameter on the dependent variables inventory and tardiness costs. This is in line with production system modeling literature stating that lot-size has a high influence on production lead time which directly influences inventory and tardiness (see Karmarkar 1987 and Altendorfer 2015). However, it also shows that both planning parameters have to be taken into account when generating a feasible surrogate model.

In Table 3 the results for these 4 surrogate modeling approaches taking both planning parameters for each material into account, i.e., 106 parameters, are presented. In general, the results show that the performance of the prediction dramatically improves. This indicates that there is a strong interaction between these two parameters and that neither parameter alone is able to explain the costs well, which is again in line with analytical findings. The comparison of the different surrogate modeling approaches identifies different approximation qualities:

- Linear regression (LR)
  - IC and TC: This approximation method leads to the worst fit for both dependent variables (see the low R^2 values). Based on these results, this method cannot be proposed for the surrogate modeling application at hand.
  - Based on the linear behavior of the approximation (see Section 4.1) and the results from analytical production literature on the non-linear relationships in production systems (see Section 1), this is an intuitive result.
- Random forest (RF)

Table 3: Model accuracies using both lot-sizes and planned lead times.

		INVENTORY COSTS (IC)			TARDINESS COSTS (TC)		
		R^2	MAE	MRE	R^2	MAE	MRE
LR	**training**	0.6907	715.04	0.0466	0.6907	13,329.08	0.5737
	test	0.6857	764.73	0.0500	0.6655	14,223.26	0.5897
RF	**training**	0.9143	411.52	0.0268	0.9560	5,202.04	0.2025
	test	0.8363	587.79	0.0384	0.9141	7,257.49	0.2703
RT	**training**	0.8860	386.06	0.0244	0.9355	5,326.46	0.1612
	test	0.8816	423.08	0.0267	0.9170	6,407.63	0.1966
GBT	**training**	0.9705	228.47	0.0147	0.9788	3,531.73	0.1265
	test	0.8956	443.30	0.0286	0.9216	6,717.87	0.2453

  - IC: This model provides a good fit for the training samples ($R^2 = 0.91$), however the fit for the test samples is not as good ($R^2 = 0.84$).
  - TC: Again, good model accuracy for the training samples can be observed, even higher than for IC. The accuracy of the test prediction is slightly lower.
  - In general, the method provides an acceptable performance.
- Regression tree (RT)
  - IC: Even though the performance within the training partition in terms of R^2 is worse than for RF and GBT, good test results for R^2 as well as MAE and MRE show that this method is one of the best.
  - TC: The model achieves similar results like for IC, but is not as good during test as in training.
  - In general, the good performance of this method can be explained because this method splits the solution space into small slices which are linearized and therefore approximate the non-linear production logistical behavior.
- Gradient boosted trees (GBT)
  - IC and TC: The method provides an excellent fit for the training samples ($R^2 = 0.97$ and $R^2 = 0.98$), however, a lower performance for the test samples ($R^2 = 0.90$ and $R^2 = 0.92$) is observed.
  - In general, the R^2 performance of this method in the test partition is still the best of all methods, nevertheless, the slightly worse MAE and MRE performance suggest that it might be better to apply RT here.

To better understand the approximated values when applying these regression methods for surrogate modeling, Figure 5 shows the scatter plots from the best models whereby results from the training set are yellow and results from the test set are orange. Looking at the results of RF and GBT shows that the estimation quality depends on the absolute value of the costs. It can be observed that higher costs are underestimated and lower costs are overestimated. This effect is more pronounced for the test samples. For RT only a slight underestimation of high costs can be observed but no overestimation of low costs.

In general, these results lead to the suggestion that the methods RF, RT and GBT can all be applied for surrogate modeling, however, the results of RT are better in the sense of cost estimation bias. The slightly lower estimation performance of RT in comparison to RF and GBT for high costs is compensated by the fact that in the surrogate models specifically low costs should be estimated well to identify possible solution candidates to be simulated. Parameter sets with high cost estimates will usually not further be evaluated.

For further simulation-based solution heuristic improvement, an interesting issue is the influence of single planning parameters on the objective function, i.e., sum of inventory and tardiness costs. An in depth

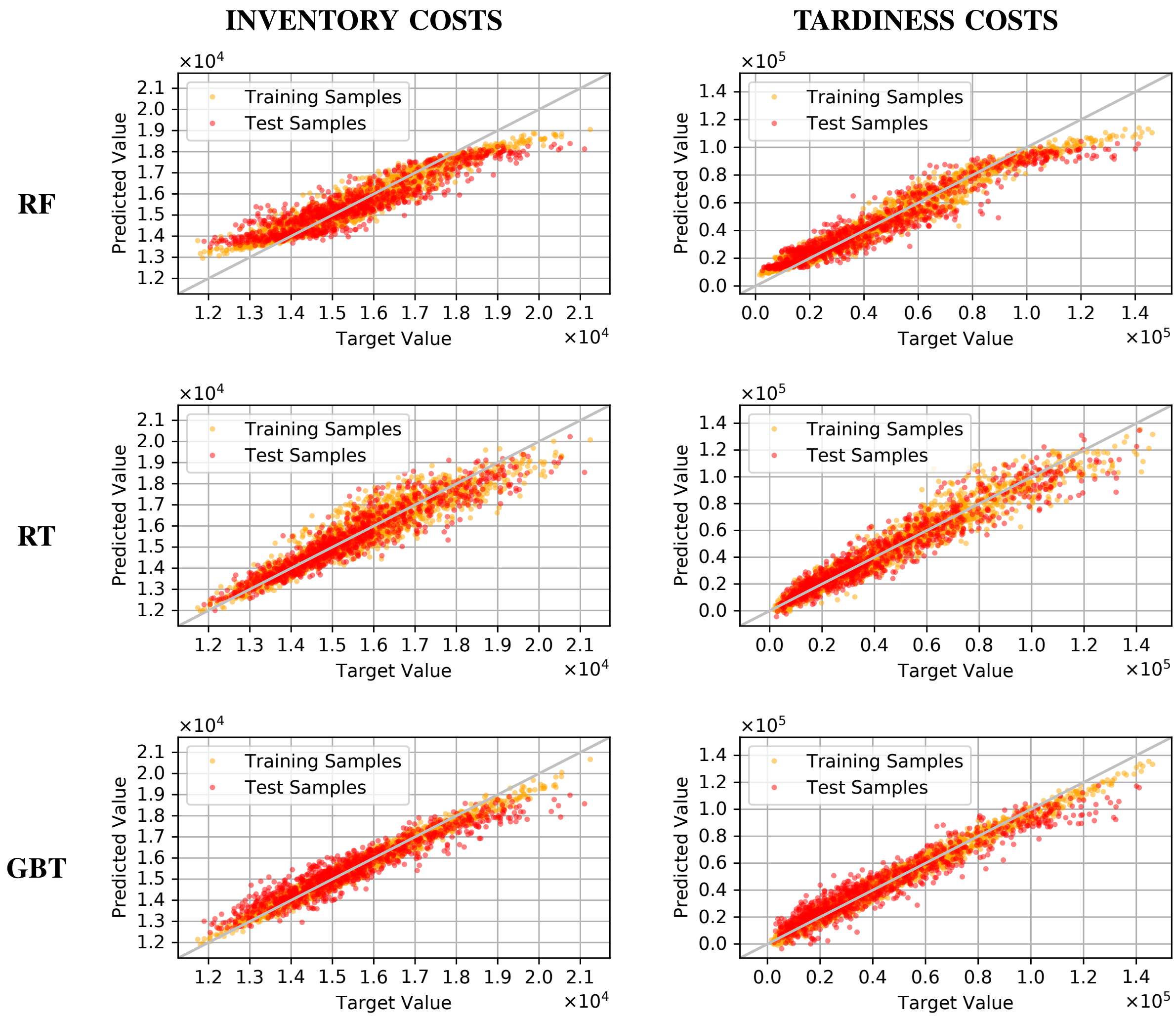

Figure 5: Scatter plots depicting the accuracy of all models.

analysis of the surrogate model results in evaluating the influence of single planning parameters on the R^2 performance has been conducted. In this simple analysis, each planning parameter's impact is evaluated by applying the regression model to the original dataset for all other planning parameters and randomized assignment of the respective parameter values. The reduction in the R^2 value between the original model and the model with randomized parameter assignment for the evaluated parameter is calculated and a higher R^2 reduction indicates a higher parameter influence. The detailed results omitted in this paper show that in all regression models only two planning parameters (planned lead time and lot-size of one material) have a very strong impact (see https://dev.heuristiclab.com/AdditionalMaterial). Thus, the costs in this simulated real-world production plant are highly dependent on the dispatching of a single material which is a valuable insight also for a simulation-based optimization heuristic.

6 CONCLUSION

In this paper the application of 4 different regression methods, i.e., linear regression, random forest, regression tree, and gradient boosted trees, for surrogate modeling in simulation-based optimization of a real production system is investigated. Based on a simulation model of a real production system, the regression models are applied to estimate the effect of lot-size and planned lead time on the inventory and tardiness costs. Linear regression does not perform well, which is in line with analytical results showing that these parameter influences are non-linear. The results for the other three regression methods are promising and provide a sufficient fit for application as surrogate models. In detail, the regression tree method performed best in this study and is therefore suggested for application. Even though the random forest and the gradient boosted trees show a better R^2 performance in the training sample and partially also in the test sample, the performance in the test sample for mean absolute error (MAE) and mean relative error (MRE) are worse. Furthermore, random forest and the gradient boosted trees both partially lead to a bias for low and high cost estimates, i.e., low costs are overestimated and high cost are underestimated.

In further research we plan to apply this regression model for surrogate model supported simulation-based optimization of real production systems. In detail the number of simulation runs to initialize the surrogate model could be investigated. With surrogate model supported simulation-based optimization the solution quality improvement can be compared to simulation model results and a simulation time reduction in comparision to a traditional grid search procedure can be studied.

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