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1 2

#### Development of a two-stage ship fuel consumption prediction and reduction model for a dry bulk ship

3

#### 4 Abstract

5 Shipping industry is the backbone of global trade. However, the large quantities of 6 greenhouse gas emissions from shipping, such as carbon dioxide (CO<sub>2</sub>), cannot be 7 ignored. In order to comply with the international environmental regulations as well as 8 to increase commercial profits, shipping companies have stronger motivations to 9 improve ship energy efficiency. In this study, a two-stage ship fuel consumption 10 prediction and reduction model is proposed for a dry bulk ship. At the first stage, a fuel 11 consumption prediction model based on random forest regressor is proposed and 12 validated. The prediction model takes into account ship sailing speed, total cargo weight, 13 and sea and weather conditions and then predicts the hourly fuel consumption of the 14 main engine. The mean absolute percentage error of the random forest regressor is 15 7.91%. At the second stage, a speed optimization model is developed based on the 16 prediction model proposed at the first stage while guaranteeing the estimated arrival 17 time to the destination port. Numerical experiment on two consecutive-8-day voyages 18 shows that the proposed model can reduce ship fuel consumption by 2% to 7%. The 19 reduction in ship fuel consumption will also lead to lower CO<sub>2</sub> emissions.

20

21 Keywords: Fuel consumption prediction, Ship fuel efficiency, Ship speed optimization,

22 Random forest regressor; Machine learning

#### 23 1. Introduction

24 In the past few years, improving ship energy efficiency has received wide attention 25 not only from governmental and non-governmental organizations, but also from 26 shipping companies (Yang et al., 2019). Although shipping is a vital component of 27 global economy, air pollutants and greenhouse gas emissions from shipping industry 28 caused by fuel consumption cannot be ignored. Regarding greenhouse gas emissions, 29 such as CO<sub>2</sub>, it is reported by the International Maritime Organization (IMO) that CO<sub>2</sub> 30 emissions from shipping constitute 3.1% of global emissions, while international 31 shipping emissions take up for 2.6% of the global emissions during 2007 to 2012 (IMO 32 2014). Thus, an increasing number of international regulations have been focused on 33 improving ship energy efficiency. The first related international regulation is the 34 amendments of the International Convention for the Prevention of Pollution from Ships 35 (MARPOL) Annex VI proposed by Marine Environment Protection Committee (MEPC) 36 in 2011 (IMO 2011). In addition, an approach named "Energy Efficiency Operational 37 Indicator (EEOI)" was also proposed as a monitoring tool to manage ship and fleet 38 efficiency performance. In 2016, amendments to MARPOL Annex VI mandatorily 39 required ships to record and report their fuel oil consumption.

40 For shipping companies, due to high fuel prices, fuel costs have become the 41 dominant factor of ship operational costs (Du et al., 2019). It is estimated that ship fuel 42 costs constitute 20% to 50% of the total ship operating costs (Leifsson, 2008; Hasselaar, 43 2011). For a large container ship, fuel costs can reach about three-quarters of its 44 operating costs when the fuel prices are high. In addition, the costs can be higher if the 45 container ship chooses to use cleaner fuel (Ronen, 2011). In shipping industry, slow 46 steaming is a commonly used countermeasure to reduce fuel consumption, but on-time 47 delivery may not be guaranteed (Lee et al., 2015). Thus, in order to conform to the 48 international environmental protection regulations as well as to increase revenue and 49 enhance competitiveness, shipping companies are developing stronger motivations to 50 propose practicable measures to increase ship energy efficiency.

51 For the existing ships, it can be hard to change their structure to reduce fuel 52 consumption. Thus, finely planning ship voyages, e.g., adopting weather routing and 53 optimizing sailing speed are more popular measures. For the fixed sailing routes over a 54 voyage, one main duty for the shipping company is to plan the daily sailing speeds of 55 the ships in advance to minimize fuel consumption over the voyage while guaranteeing 56 on-time arrival. Sailing speed optimization requires predicting ship fuel consumption 57 in different situations. However, there are several challenges in making accurate 58 prediction. First, inaccuracy exists in ship sailing data that can be used to construct fuel 59 consumption prediction models, as these datasets mainly come from manually filled 60 ship log data, such as noon reports. Second, factors influencing ship fuel consumption

61 are high-dimensional. Although it is widely believed that ship sailing speed is the most 62 important influencing factor on ship fuel consumption (Fagerholt et al., 2010; Corbett 63 et al, 2009; Psaraftis and Knotovas, 2013, Bialystocki and Konovessis, 2016), other 64 factors can also have impacts. These factors include but are not limited to trim condition, 65 displacement and draft conditions, weather and sea conditions, and hull and propeller 66 roughness (Andersen et al., 2005; IMO, 2011; Bialystocki and Konovessis, 2016). 67 Nevertheless, it is hard to have detailed information on all the influencing factors on 68 fuel consumption, which prevents classic regression models from making accurate fuel 69 consumption prediction. Third, as different ships have different properties and 70 structures, one fuel consumption prediction model cannot be universally applied 71 (Banawan et al., 2013). Alternatively, a tailored prediction model should be developed 72 for each single ship to achieve more satisfactory prediction performance. Developing 73 tailored machine learning models is a desirable and promising way to deal with these 74 challenges. Machine learning models have the ability to handle multi-dimensional input 75 data and to extract hidden information from complex datasets. In addition, they usually 76 have better ability to deal with noisy data. Compared with traditional statistical 77 regression models, machine learning models can address higher dimensional data (e.g., 78 ship displacement conditions, sea and weather conditions, trim conditions, and sailing 79 speed) and make much more accurate predictions, and thus provide a more reliable 80 foundation on developing tailored ship fuel consumption reduction models.

The purpose of this study is to propose a two-stage ship sailing speed optimization model for a dry bulk ship which contains two steps: in step 1, a machine learning model performing regression task (i.e. a random forest regression model) with high accuracy is proposed to make predictions on ship fuel consumption under different sailing speeds as well as cargo, weather, and sea conditions; in step 2, a sailing speed optimization model is proposed based on the prediction results in step 1 to minimize ship total fuel consumption over a voyage.

88

#### 89 2. Literature review

### 90 2.1 Research on ship fuel consumption prediction

91 During the last few years, there has been an increasing amount of literature on 92 prediction of ship fuel consumption (Zhao and Yang, 2018; Yang et al., 2019). The 93 pioneering, basic, and commonly used models are deterministic models, which are also 94 called white box models. In a deterministic model, the ship behavior of hull resistance, 95 propeller propulsion, and main engine performance are described (Yang et al., 2019). 96 Typical and pioneering studies include Holtrop (1977, 1978), Holftrop and Mennen 97 (1978), and modern studies include Kristensen and Lützen (2012). Apart from the 98 deterministic model, two types of models are also widely used in more recent research:

99 statistical models and machine learning models. Regarding the development of 100 statistical models for fuel consumption prediction, Bocchetti et al. (2013) proposed a 101 multiple linear regression analysis model, which took ship sailed distance and 102 displacement as well as wind speed conditions into account to predict fuel consumption 103 and CO<sub>2</sub> emissions of a cruise ship. Bochetti et al. (2015) then developed another 104 multiple linear regression model for a cruise ship by containing more influencing 105 factors. Erto et al. (2015) also developed a multiple linear regression model for a cruise 106 ship by taking ship operational factors and wind condition into consideration. As the 107 foundation of a ship fuel consumption analysis system, Kee et al. (2018) proposed a 108 multiple linear regression method to estimate fuel consumption of two tugboats. 109 Although statistical models are intuitive and interpretable, there can be some drawbacks. 110 First, parametric statistical models require making assumptions on data distributions 111 before developing models, and this may bring bias. In addition, even if the log-log 112 model can express the power function of speed and fuel consumption, the linear 113 regression models usually cannot perform well when dealing with complicated data and 114 multicollinearity data. Moreover, they are easily influenced by noisy data (Neter et al., 115 1996; Goldstein, 2011).

116 Over the past years, a growing body of innovative literature has focused on 117 developing machine learning methods for ship fuel consumption prediction. The most 118 popular method is Artificial Neural Networks (ANNs) model. Pedersen and Larsen 119 (2009) proposed an ANN model for predicting propulsion power of a tanker based on 120 ship noon report data. They also found that by combining sea and wind information, 121 the performance of ANN model could be significantly improved. Besikci et al. (2016) 122 developed a decision support system (DSS) for improving energy efficiency of an oil 123 tanker. The decision system contained two parts: an ANN model for fuel consumption 124 prediction under various operational conditions and a DSS based on the prediction 125 results for energy-efficient ship operations. In comparison studies, they reported that 126 the performance of the ANN model was superior to multiple regression analysis based 127 on their dataset. Petersen and Jacobsen (2012a) compared the performance of ANN and 128 Gaussian processes (GP) models when applied to predict fuel consumption of a 129 domestic ferry. The result indicated that the performance of ANN was a little superior 130 than the GP in all the tests. Petersen et al. (2012b) proposed tapped-delay neural 131 network model for fuel consumption prediction of a tanker, which was then applied to 132 trim optimization of the tanker. Petursson (2009) developed five machine learning 133 models for fuel consumption prediction of a passenger ship: support vector regression 134 (SVR), k-nearest neighbor (kNN), ANN, classification and regression trees (CART) 135 and bagging. They found that the SVR and kNN outperformed the other models on their 136 dataset. Other types of machine learning models are also adopted for ship fuel

137 consumption prediction. A least absolute shrinkage and selection operator (LASSO) 138 regression model, which contained sea and weather conditions, was adopted to predict 139 fuel consumption of a container ship (Wang et al., 2018). Soner et al. (2018) developed 140 three tree-based models: bagging, random forest, and bootstrap based on the log dataset 141 of a ferry ship that was also used by Petersen et al. (2012b). They identified that the 142 performance of tree-based prediction models had higher prediction accuracy. Grey-box 143 models, which is in between the white-box model and black-box model, were also 144 developed. More specifically, one type of the grey-box model structure is built based 145 on basic principles of ship propulsion and the unknown parameters are estimated by 146 statistical regression models, such as Journée et al. (1987), Lu et al. (2013), Meng et al. 147 (2016) and Yang et al. (2019). The other type of grey-box model combines white-box 148 model, which describes some components of resistance or fuel consumption, and black-149 box model, such as machine learning and statistical models, for the remaining parts. 150 This type of grey-box model can be seen in Leifsson et al. (2008), Coraddu et al. (2015), 151 Haranen et al. (2016), and Coraddu et al. (2017). The advantage of grey-box models is 152 they are able to integrate mechanistic knowledge with data analysis methods.

Machine learning models are capable of dealing with high-dimensional data and making more accurate predictions on complicated data than traditional regression models. In addition, no human interventions are needed when learning the models (Bishop, 2006; Alpaydin, 2009). Several studies have shown that the machine learning models outperform statistical models (Petersen and Jacobsen, 2012a; Wang et al., 2018; Du et al., 2019).

159 Regarding the factors that influence ship fuel consumption, almost all the above-160 mentioned studies, either based on statistical regression methods or machine learning 161 methods, show that ship sailing speed is the dominant factor for ship fuel consumption 162 prediction (Bocchetti et al., 2013, 2015; Petersen and Jacobsen, 2012a; Meng et al., 163 2016). Actually, the "cubic law" between ship sailing speed and fuel consumption, i.e., 164 the bunker consumption of a ship in one time unit is proportional to the sailing speed 165 to the power of three, is widely-believed and adopted in shipping industry and maritime 166 studies (Meng et al., 2016). Apart from sailing speed, ship displacement, such as total 167 weight of the ship, cargo conditions, and ballast water, can also have an influence on 168 fuel consumption based on vessel dynamics. Sea conditions, such as ocean currents (Lo 169 and McCord, 1995), sea waves and swell (Lu et al., 2015; MAN Diesel & Turbo, 2011), 170 are also proved to be influential to ship fuel consumption. Moreover, weather conditions 171 are regarded as relevant to ship fuel consumption. For example, Kwon (1981) and 172 Townsin and Kwon (1993) investigated weather conditions on ship performance and a 173 group of regression models were proposed. Recently, models incorporating sea and 174 weather information, including wind direction and force, sea wave direction and height,

and sea water temperature have exhibited high accuracy in ship fuel consumption
prediction, such as the models proposed by Wang et al. (2016), Lee et al. (2018), Meng
et al. (2016), and Du et al. (2019). Combining ship sailing related features together with
sea and weather conditions have shown great potential in ship fuel consumption
prediction and management.

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## 181 **2.2 Research on improving ship energy efficiency**

182 Much of the current literature on ship energy efficiency pays particular attention to 183 finding viable measures to reduce ship fuel consumption. As suggested by SEEMP, 184 there are several effective ways to save ship fuel consumption from management 185 perspective, which mainly include speed optimization, weather routing, efficient cargo 186 operation, and trim optimization. As sailing speed is the most significant influencing 187 factor, a considerable amount of literature has been focused on optimizing ship sailing 188 speed to reduce fuel consumption, such as Fagerholt et al. (2010), Norstad et al. (2011), 189 Yao et al. (2012), Wang and Meng (2012), Wang et al. (2013), Lee et al. (2015), 190 Lindstad and Eskeland (2015), Song et al. (2015), Wang (2016) and Wang and Wang 191 (2016). Weather routing helps ships to locally avoid rough sea and weather conditions 192 in order to guarantee sailing safety as well as reduce fuel consumption. Studies on 193 designing ship routes over a voyage based on weather information to realize fuel 194 consumption reduction include Takashima et al. (2009), Shao et al. (2012), and Lin et 195 al. (2013). IMO reported that trim optimization could reduce the main engine fuel 196 consumption for most ship types by 0.5% to 3.0% (IMO, 2019). There is also research 197 on developing trim optimization schemes for ship fuel consumption reduction, such as 198 Reichel et al. (2014), Sherbaz and Duan (2014), Perera et al. (2015), and Moustafa et 199 al. (2015). Proposing efficient ship cargo operation is often combined with fleet 200 deployment and speed optimization, e.g., Xia et al. (2015) and Wang et al. (2015).

201 Over the period from 2016 through 2019, much more attention has been focused 202 on developing two-phase optimization models for ship energy efficiency improvement. 203 Generally, in the first phase, one or more models are developed for fuel consumption 204 or weather conditions prediction under different situations; in the second phase, an 205 optimization model is proposed for ship fuel consumption reduction over a voyage. 206 Some typical two-phase models are presented as follows. Wang et al. (2016) proposed 207 a real-time optimization model for a cruise ship which contained prediction of weather 208 condition based on wavelet neural network (WNN) and determining the optimal engine 209 speed based on the calculated ship resistance. Coraddu et al. (2017) developed a vessel 210 trim optimization model for a tanker ship. The model included two parts: in the first 211 part, a grey box model, which contained both mechanistic knowledge and historical 212 data analysis, was proposed to predict the fuel consumption; in the second part, trim 213 optimization techniques were proposed. Lee et al. (2018) proposed a way to explore 214 weather archive big data and optimize sailing speed for a container ship. First, the 215 impact of weather conditions on ship fuel consumption was figured out by data mining 216 methods. Then, speed optimization model was developed for the container. Du et al. 217 (2019) presented a two-phase model for speed and trim optimization for a container. In 218 the first phase, an ANN model was developed for estimating ship fuel consumption in 219 different conditions. In the second phase, three countermeasures were put forward for 220 reducing fuel consumption, including speed optimization, trim optimization as well as 221 speed and trim optimization.

222 Although there are a growing number of studies on predicting and reducing ship 223 fuel consumption, there are still considerable gaps existing in current literature. First, 224 the literature has studied tankers, container ships, ferries, tugboats, and passenger ships. 225 However, to the best of our knowledge, no model containing machine learning 226 techniques for fuel consumption prediction and speed optimization are proposed for dry 227 bulk ships. As the fuel prediction and optimization models are not universally applied 228 (Lee et al., 2018; Banawan et al., 2013), it is necessary to develop such tailored model 229 for a specific dry bulk carrier. Second, a large number of studies only include ship 230 sailing speed as the input feature to predict ship fuel consumption. Actually, the 231 determinants of fuel consumption are varied, including ship displacement and trim 232 conditions as well as sea and weather conditions, but there is only a small number of 233 studies considering these factors. Even if some studies take sea and weather information 234 into account, the information is taken just from the noon report. Few studies have 235 combined ship noon report with weather forecast, which could provide more 236 comprehensive and accurate data. Third, most of the proposed machine learning models 237 for ship fuel consumption prediction are based on ANNs. However, the development of 238 ANN models usually requires a large number of training samples, and their structures 239 are largely based on experience. In addition, tuning the parameters in ANNs can be 240 difficult, and the prediction results are lack of interpretability. Moreover, the 241 influencing degree of each input variable on the output variable is hard to figure out. 242 Fourth, there are only a few pioneering studies on combining ship fuel prediction 243 models and optimization models that can be put into practice to reduce fuel 244 consumption and CO<sub>2</sub> emissions.

To bridge the gaps, we propose a two-stage model for a dry bulk ship based on ship noon report data and weather forecast data that contains (i) prediction of ship fuel consumption under different sailing speed, cargo, wind, swell, wind waves, and current conditions by adopting a random forest regressor, which is an ensemble learning method for regression based on multiple decision trees, and (ii) development of a speed optimization model to minimize ship fuel consumption over a voyage while guaranteeing the estimated arrival time to the destination port based on the prediction results at the first stage. Compared with traditional statistical regression models, the advantages of using random forest regressors are that they are able to deal with highdimensional data and make more accurate predictions. Compared to some other machine learning models, including ANNs, they are easier and faster to be implemented with more interpretable results and the influence degree of the features on the target variable can be generated, which can be used for feature selection.

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#### 259 **3. Data description**

## 260 3.1 Ship noon report

261 Noon report of a ship is a ship voyage report data sheet prepared by the ship's 262 captain on a daily basis (usually at noon). Many attributes of the ship's sailing behavior 263 are recorded, such as ship geographic location, distance travelled since last report, 264 average propeller revolutions per minute (RPM), engine speed, sailing speed, total hold 265 cargo and total deck cargo. In addition, sea and weather conditions of the recording 266 time are also comprised, e.g., information on sea swell direction (coming direction of 267 sea swell), sea swell height, sea current value (depth of sea current), sea current type 268 (coming direction of sea current), wind force, wind direction (coming direction of wind), 269 and sea temperature. It should be noted that although noon report data is the main source 270 for ship fuel consumption and optimization research, the features contained in the report 271 are limited and may vary among different reports. The factors used in other studies that 272 also choose noon report as the data source for ship fuel consumption management are 273 similar, such as "wind speed and direction, sea water temperature, air temperature, 274 water depth, and wave height and direction" in the model calibrated by Pedersen and 275 Larsen (2009), "displacement, wave direction and height, and wind force" in the model 276 proposed by Meng et al. (2016), "displacement, wave direction, wind force and 277 direction, sea current direction, sea water temperature, and trim" in the model 278 developed by Du et al. (2019), "forward draft, aft draft, wind direction and wind 279 Beaufort number" in the model presented by Yang et al. (2019).

280 **3.2 Description of ship voyage data** 

281 The voyage data used in this study is the noon report data of a handy-size dry bulk 282 ship with propeller diameter 5450mm, which was provided by an international shipping 283 company. Time range of the voyage data is from 11<sup>th</sup> September 2017 to 27<sup>th</sup> February 284 2019. Initially, the voyage report data for the ship contains 738 data entries. To start 285 with, we filter the data entries by choosing the records with ship conditions as "sailing 286 at sea", "with cargo loaded" and sailing speed value no less than 5 knots. After 287 preprocessing, there are 242 selected entries left in the entire case dataset. Then, we use 288 the hourly fuel consumption of the ship as the target variable (which is calculated by

289 dividing the total fuel consumption by the total steaming hours) and delete the variables 290 that are not suitable to be the input of the fuel consumption prediction model. Finally, 291 9 input variables are selected from the attributes in the voyage data, namely, bad 292 weather ratio, ship sailing speed (knots), relative sea swell direction to ship's heading 293 (°), sea swell height (m), sea current type, sea current value (m), relative wind direction 294 to ship's heading (°), wind force (Beaufort force number), and total cargo weight 295 (metric ton). Based on the recording time and location (longitude and latitude) provided 296 by the noon report, we include two more attribute variables: height of combined wind 297 waves and swell (m) and relative wind wave direction to ship's heading (°) downloaded 298 from the European Centre for Medium-Range Weather Forecasts (ECMWF) (ECMWF, 299 2019). Eventually, the dataset contains 11 features as the input. Table 1 presents the 300 statistical information of the variables in the case dataset. Figure 1 illustrates the 301 distributions of the 242 data entries for the selected ship against the 11 input variables 302 and the output variable.

303

#### Table 1. Description of the variables in the entire dataset

Variable name	Meaning	Unit	Max value	Min value	Mean value
Hourly main engine fuel consumption	Fuel consumption of main engine in an hour	MT/h	0.9275	0.4139	0.7064
Bad weather ratio	Steaming time in bad weather/total steaming time	\	1	0	0.4139
Sailing speed	Ship average sailing speed	knots	14.2	5.3	11.1021
Relative sea swell direction	Direction of sea swell relative to ship's heading degree (-1 for no swell)	degree	180	1	87.3440
Sea swell height	Height of sea swell	meter	4	0	1.9959
Sea current type	Sea current against ship's heading $(-1)$ , with ship's heading $(+1)$ , no current $(0)$	X	1	-1	-0.3843
Sea current value	Depth of sea current	meter	4	0	0.4628
Relative wind direction	Direction of wind relative to ship's heading degree (-1 for no wind)	degree	180	0	99.8333
Wind force	Measure of wind speed	Beaufor force number	t 8	0	4.9008
Total cargo weight	Sum of the weights of on-deck cargo and under-deck cargo	MT	32741.5	11260	28685.06
Combined wind	Height of the combination of wind	meter	9	0.1	2.1406
waves and swell height	waves and swell (-1 for no wave and swell)				
Relative wind wave direction	Direction of wind wave relative to ship's heading degree (-1 for no wave)	degree	179	0	81.1972









(a) Distribution of hourly main engine

fuel consumption

(c) Distribution of ship sailing speed



(e) Distribution of sea current type and sea current value



(g) Distribution of total cargo weight

(b) Distribution of bad weather ratio



(d) Distribution of relative sea swell direction and sea swell height



(f) Distribution of relative wind direction and wind force



(h) Distribution of combined wind waves and swell height



(j) Distribution of relative wind wave

direction

Figure 1. Distribution of data entries in the entire dataset

In order to validate the performance of the proposed two-stage speed optimization model for ship fuel consumption reduction, we randomly select two 8-day continuous noon report data from the entire dataset which is used for numerical experiments. The noon report records from 16 Jan 2018 to 23 Jan 2018 and from 24 Dec 2018 to 31 Dec 2018 are selected, respectively. For the remaining 226 data entries, 80% of them are randomly selected to constitute the training set to develop the regression models, while the remaining 20% form the test set.

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#### **4.** Development of tree-based models for ship fuel prediction

#### 4.1 Introduction of Decision tree (DT) regression model

316 A decision tree (DT) is a supervised and tree-like decision support model which is 317 widely used to predict both discrete valued output (*classification tree*) and continuous 318 valued output (regression tree) (Myles et al., 2004). There are several nodes in a 319 decision tree, and each node contains a certain number of input data entries. The output 320 value of a node is the average output of all the comprised data entries. A decision tree 321 consists of three types of nodes: root node (the topmost node), leaf node (which gives 322 final prediction output), and internal node (node except for root and leaf node). The 323 process of dividing a node into two successive nodes is called *splitting*. A feature and 324 one of its corresponding value are chosen to split a node, and each splitting of a node 325 requires finding out the best split based on some splitting criteria. In DT classifiers, 326 common splitting criteria are Gini impurity and information gain. In DT regressor, 327 common splitting criterion is mean squared error (MSE) (Friedman et al., 2001). A 328 node being split is called parent node while the successive nodes are called child nodes.

Three widely used DT generation algorithms are ID3, C4.5, and CART (Classification and Regression Tree) (Loh, 2014). As both input and output data contain continuous valued data, we construct a DT regressor by adopting CART algorithm (Breiman et al., 1984). CART algorithm requires recursively and binarily splitting the

- nodes, and a binary decision tree will be built. Originally, the construction process
  terminates when all the leaf nodes contain the data entries of the same output value.
  However, this usually means that the tree is extremely large and is heavily overfitted.
  To alleviate overfitting, termination criteria are preset to control tree dimension. Three
  commonly used criteria are presented as follows. It should be noted that the values of
  these decision tree parameters may vary from different training sets.
- (a) The maximum depth of a tree (denoted by *max\_depth*). The depth of a node in a
  decision tree is the number of nodes on a route from the root node to its parent node
  (the depth of root node is 0). The maximum depth of the tree is the maximum depth of
  all the nodes. A node cannot be further split if it reaches the maximum depth.
- 343 (b) The minimum number of data entries required to split a node (denoted by
  344 *min\_samples\_split*). If and only if a node contains data entries no less than
  345 *min\_samples\_split* can this node be further split.
- (c) The minimum number of data entries required to be at a leaf node (denoted by *min\_samples\_leaf*). If and only if the number of data entries contained in both of the
  successive nodes split by the *best split* is no less than *min\_samples\_leaf* can the node
  be split.
- Learning an optimal decision tree is known as an NP-complete problem (Laurent and Rivest, 1976; Naumov, 1991). Starting from splitting the root node, successive nodes are split in a depth-first manner until one of the termination criteria has been reached. Then, the next node for splitting is determined by retrospectively search for a node that can be further split. The algorithm terminates until there is no node that can be split. Main steps to generate a decision tree are described in Appendix A (Friedman et al., 2001; Harrington, 2012; Breiman, 2017).

## **4.2 Introduction of random forest (RF) regression model**

358 Although the DT models are simple, intuitive, and interpretable, the main 359 drawbacks of a single decision tree are that they are easy to get overfit (i.e., creating 360 over-complex trees with poor generalization ability) and lack of robustness (i.e., small 361 variations in the training data might result in a completely different tree being generated) 362 (Ahmad et al., 2017). Ensemble learning is one of the popular ways to improve DT 363 regressor performance. Ensemble methods contain multiple learning algorithms (called 364 weak learners) and can obtain more desirable predictive performance than any of the 365 constituent learning algorithms alone (Opitz and Maclin, 1999). There are two popular 366 ensemble methods based on decision trees: boosting and bagging. In boosting, 367 successive trees are dependent on the earlier trees, while in bagging, the trees are 368 constructed using bootstrap sample of the training set (i.e., randomly selecting a certain 369 number of samples from all the training samples with replacement) and the trees are 370 independent on the other trees. Based on the bagging method, Breiman (2001) proposed

- random forests by adding another layer of randomness: instead of considering all the
  data features to split the nodes in each DT included in the forest, a randomly generated
  subset of candidate features is used. Thus, apart from the abovementioned three
  parameters in DT regressor, there are two more parameters in RF regressor:
- (d) The number of decision trees contained in the forest (denoted by *n\_estimators*).
  Breiman (2001) proposed that adding more trees in the RF regressor will not suffer
  from overfitting. Instead, more trees have the ability to limit the value of generalization
  error.
- (e) The number of features to consider when finding the *best split* of a node in each
  decision tree (denoted by *max\_features*). The value of *max\_features* should less than
  the total number of data features and the certain number of features are randomly
  selected at each splitting.

383 If CART based decision trees are the weak learners in a RF regressor, the main 384 differences between constructing a DT regressor and a single decision tree in the RF 385 regressor are twofold. (i) For a decision tree in RF regressor, bootstrap sampling from 386 the entire training set to form a new training set is required; for a normal DT regressor, 387 all the entries in the training set are used. (ii) For a decision tree in RF regressor, 388 randomly selecting a subset of data features for splitting the nodes in each decision tree 389 is required; for a normal DT regressor, all the features are considered when splitting 390 each node. After a certain number of DTs are constructed, the RF regressor requires 391 averaging the output values of all the tress as the prediction results (Liaw and Wiener, 392 2002). Compared with DT regressor, RF regressor has the advantages of robustness and 393 lower variance (Siroky, 2009). For the detailed process of constructing an RF regressor, 394 please refer to Breiman (2001), Biau and Scornet (2016), and Breiman (2017).

## <sup>395</sup> 4.3 Metrics for model validation

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In order to demonstrate the model performance in the test set, four typical regressor performance measures are adopted: *mean squared error* (MSE), *root mean squared error* (RMSE), *mean absolute error* (MAE), and *mean absolute percentage error* (MAPE). Denote the input variable vector by  $x_e$ , the predicted output value by  $f(x_e)$ , and the real output value by  $y_e$ . The total number of data entries in the test set is N. The definitions of MSE, RMSE, MAE, and MAPE are as follows:

$$MSE = \frac{1}{N} \sum_{e=1}^{N} [f(x_e) - y_e]^2$$
(1)

403 
$$RMSE = \sqrt{\frac{1}{N} \sum_{e=1}^{N} [f(x_e) - y_e]^2}$$
(2)

404 
$$MAE = \frac{1}{N} \sum_{e=1}^{N} |f(x_e) - y_e|$$
(3)

$$MAPE = \frac{100\%}{N} \sum_{e=1}^{N} \left| \frac{f(x_e) - y_e}{y_e} \right|.$$
(4)

#### 406 4.4 Construction and prediction results of DT and RF regression models

We adopt the scikit-learn machine learning library for Python to implement DT regressor and RF regressor based on CART algorithm (Pedregosa et al., 2011). The parameters for DT and RF regressors are set based on gird search method with five-fold cross validation as presented in Table 2. Except for those parameters, all the other parameters are set as the default values in scikit-learn library.

		θ
Parameter	Decision tree regressor	Random forest regressor
max_depth	4	11
min_samples_split	5	2
min_samples_leaf	10	1
n_estimators	/	1000
max_features	/	4

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Table 2. Parameters used in DT and RF regressors

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The DT regressor model is visualized in Figure 2. For each root and internal node in the figure, the first row indicates the selected splitting variable and the splitting value. The second row shows the number of samples contained in the node. The third row is the output value of this node. For each leaf node, the first row is the number of samples contained in the node, and the second row is the final output value.



- 419
- 420

Figure 2. Visualization of the DT model for ship fuel prediction

421 The prediction performance of the two proposed regression models has also been 422 compared with the popular machine learning based fuel consumption prediction 423 methods in current literature. Three typical and popular regression models are selected 424 for comparison: artificial neural network (ANN), least absolute shrinkage and selection 425 operator (LASSO) regression, and support vector regression (SVR). ANN is a widely 426 used machine learning model which contains a large number of highly interdependent 427 processing elements called neurons. Usually, a typical ANN contains three layers of 428 neurons: input layer, hidden layer, and output layer. LASSO is a linear regression 429 analysis method that can perform variable selection and regularization in order to 430 improve regression performance. SVR is an application of support vector machine 431 (SVM) to regression problems. The datasets used for training and testing the models 432 are the same as those are used for the DT and RF regressors. It is worth mentioning that 433 the LASSO and SVR models are implemented by adopting scikit-learn machine 434 learning library for Python, and the parameters for the two models are tuned by gird 435 search method with five-fold cross validation. The construction of the ANN model is 436 similar to Du et al. (2019): five ANN models are constructed in MATLAB R2017a and 437 the average of the outputs of the five ANN models is the prediction output. The 438 prediction performance of the DT regressor, RF regressor, ANN, LASSO, and SVR 439 models are on a daily basis, i.e., hourly fuel consumption data has been converted to 440 fuel consumption for a day by considering steaming hours, are shown in Table 3. It can 441 be seen that both of the tree-based regressors perform well on our test set and the RF 442 regressor performs the best. Moreover, the RF regressor outperforms the DT regressor 443 regarding every metric.

444

Table 3. Performance of the five regression models on test set

Model/Metric	MSE	RMSE	MAE	MAPE
DT regressor	6.16	2.48	1.74	11.33%
<b>RF</b> regressor	3.17	1.78	1.21	7.91%
ANN	5.67	2.38	1.68	11.95%
LASSO	5.60	2.37	1.72	11.51%
SVR	9.37	3.06	2.55	15.47%

445

#### 446 5. Development of ship speed optimization model

## 447 5.1 Problem description

As mentioned in the introduction part, shipping companies have a strong motivation to carefully plan ship sailing speed during a voyage to reduce bunker consumption and comply with the environmental protection conventions. Based on the proposed RF regressor, which is able to predict fuel consumption of the dry bulk ship under different sailing speeds, total cargo weight and sea and weather conditions, we develop a speed optimization model between two ports while guaranteeing ship estimated time of arrival (ETA) to the destination port.

To develop the sailing speed optimization model, we consider a situation when this dry bulk ship sails from an origin port A to a destination port B along a fixed path which the captain is quite familiar with. The loaded cargo of this ship is pre-determined and fixed during the voyage and the sea and weather conditions can be obtained via forecasts 5 to 7 days in advance. Due to the dynamic conditions at sea, the whole path can be divided into several segments, and in each segment, we assume that the 461 international conventions that the ship needs to obey as well as sea and weather 462 conditions can be viewed as identical. A lower bound and an upper bound of permitted 463 ship sailing speed are also the same in one segment. The range of the allowable sailing 464 speed is determined by many factors, especially the sea and weather conditions in the 465 segment. For example, Tsou and Cheng (2013) adopted a formula to calculate a ship's 466 allowable maximum speed while navigation in storm conditions based on wave height 467 and wave direction to ensure navigational safety. The ship departure time from port A 468 is 0, and the ETA of port B is no later than the latest allowable arrival time. Two 469 questions need to be addressed: when to adjust the sailing speed (referred to as the time 470 of speed turning point) and what speed should be adjusted to (referred to as adjusted 471 speed). The objective of the model is to minimize the total fuel consumption of this dry 472 bulk ship over the whole voyage by determining the sailing speed in each segment. 473 Except for sailing speed, external factors that influence ship fuel consumption are the 474 same in one segment and thus the optimal speed should be the same in a segment. Thus, 475 it can be justified that the speed turning points can only occur at the beginning of a 476 segment. An illustration of the optimization problem is presented in Figure 3.



i	Index of a path segment,	$i \in \{1, \dots, n+1\}$ . Segment	<i>n</i> +1	presents the end of
	segment $n$ , i.e., port B			

*I* Set of all path segments,  $I = \{1, ..., n\}$ 

#### 481

Parameter	S
C <sub>i</sub>	Ship total loaded cargo and sea and weather conditions in segment <i>i</i>
$v_0$	Ship speed before departure
$\mathcal{V}_{i,c_i}^{\max}$	Maximum allowable speed when sailing in segment $i$ with the loaded

cargo and sea and weather conditions as  $c_i$  (knots)

- $v_{i,c_i}^{\min}$  Minimum allowable speed when sailing in segment *i* with the loaded cargo and sea and weather conditions as  $c_i$  (knots)
- $f^{RF}(v,c)$  Predicted ship fuel consumption (ton/hour) by using the proposed RF model when sailing speed is v and ship total loaded cargo and sea and weather conditions are c
- $L_i$  Path length of segment *i* (nm)
- $T_{\text{max}}$  Latest allowable arrival time to the destination port

482

Main dec	vision variables
<i>v</i> <sub>i</sub>	Ship sailing speed in segment <i>i</i> (knots)
Auxiliary	decision variable
t <sub>i</sub>	Arrival time to the beginning of segment <i>i</i> , $t_1 = 0$ . $t_{n+1}$ is the arrival time
	to the end of segment $n$ , i.e., the arrival time of port B.

The speed optimization problem can be formulated by using Model M1 based on
the parameters and decision variables.

<sup>485</sup> [M1]

486

488

$$\min\sum_{i=1}^{n} (f^{RF}(v_i, c_i) \times \frac{L_i}{v_i})$$
(5)

487 subject to:

$$t_{i+1} = t_i + \frac{L_i}{v_i}, \forall i \in I$$
(6)

- $t_{n+1} \le T_{\max} \tag{7}$
- 490  $v_0 = 0$  (8)
  - $v_{i,c_i}^{\min} \le v_i \le v_{i,c_i}^{\max}, \forall i \in I$ (9)
- 492

491

$$t_i \ge 0, \,\forall i \in I \bigcup \{n+1\}.$$

$$(10)$$

Objective (5) minimizes ship fuel consumption over the voyage. Constraint (6) 493 494 indicates the relationship between the arrival time to the beginning of the previous segment and that of the next segment. Constraint (7) ensures the ship arrival time to the 495 496 destination port is no later than the allowable arrival time. Constraint (8) ensures the sailing speed before departure is 0. Constraint (9) guarantees the lower and upper 497 bounds of the sailing speed in each segment. Constraint (10) grantees that the arrival 498 499 time to the beginning of every segment is nonnegative. M1 cannot be solved directly by the off-the-shelf optimizers, thus we linearize the model in the next section. 500

#### 501 5.3 Linearization of model M1

502 Given the maximum and minimum allowable sailing speeds, we can discretize the 503 speed values with 0.1 knot as an interval. Specifically, given  $v_{i,c_i}^{max}$  and  $v_{i,c_i}^{min}$  in segment 504 i respectively, as we discretize the sailing speeds with 0.1 as an interval, we have the 505 sailing speed parameters  $v_i^1 = v_{i,c_i}^{\min}$ ,  $v_i^2 = v_i^1 + 0.1$ ,...,  $v_i^{u_i} = v_{i,c_i}^{\max}$  and a specific sailing 506 speed as  $v_i^u = \{v_i^1, v_i^2, ..., v_i^{u_i}\}$ . We further introduce a binary decision variable  $y_i^u \in \{0,1\}$ , 507 and if  $v_i = v_i^u$ ,  $y_i^u = 1$ ; otherwise  $y_i^u = 0$ . The new main decision variable is  $y_i^u$ , and the 508 auxiliary decision variable is  $t_i$ . Based on the new parameters and decision variables, 509 we can convert model M1 to model M2. 510 [M2]

511 
$$\min \sum_{i=1}^{n} \sum_{u=1}^{u_i} [y_i^u \times (f^{RF}(v_i^u, c_i) \times \frac{L_i}{v_i^u})]$$
(11)

512 subject to:

513 
$$t_{i+1} = t_i + \sum_{u=1}^{u_i} (\frac{L_i}{v_i^u} \times y_i^u), \forall i \in I$$
(12)

$$t_{n+1} \le T_{\max} \tag{13}$$

515 
$$v_0 = 0$$
 (14)

516 
$$y_i^u \in \{0,1\}, \forall i \in I, u \in \{1,2,...,u_i\}$$
 (15)

517 
$$\sum_{u=1}^{u_i} y_i^u = 1, \forall i \in I$$
 (16)

518

$$t_i \ge 0, \,\forall i \in I \cup \{n+1\} \tag{17}$$

Model M2 is equivalent to M1 and is a mixed-integer linear programming (MIP)
model, which can be solved by the off-the-shelf optimizers, such as CPLEX.

521

#### <sup>522</sup> 6. Computational experiments

### <sup>523</sup> 6.1 Prediction of ship fuel consumption

524 In this section, we adopt the RF regressor developed in Section 4 to predict fuel 525 consumption of the dry bulk ship during two continuous 8-day sailing voyages (denoted 526 by voyage 1 and voyage 2, respectively). The total sailing distance of voyage 1 is 2001.2 527 nautical miles with the total sailing time as 195 hours, and the total fuel consumption 528 is 126.36 tons. The total sailing distance of voyage 2 is 1946.4 nautical miles with the 529 total sailing time as 192 hours, and the total fuel consumption is 114.92 tons. The total 530 cargo weight as well as sea and weather conditions in each sailing segment of each 531 voyage are presented in Table 4 and Table 5.

Table 4. Initial ship sailing information of voyage 1

	Day	Steaming hour (h)	Total fuel (tons)	Speed (knots)	Hourly fuel consumption (tons/h)	Bad weather ratio	Relative sea swell direction (degree)	Sea swell height (m)	Sea current type	Sea current value	Wind force (Beaufort force number)	Relative wind direction (degree)	Total cargo weight (MT)	Combined Wind Waves and Swell Height	Relative Wind Wave Direction (degree)
E 2 2	1	24	15.69	10	0.65375	1	160	2	0	0	6	160	26605	(m) 1.7	136
555	2	24	15.42	9.9	0.64250	1	89	2	0	0	6	111.5	26605	3.0	92.3
	3	25	16.22	9.8	0.64880	0.40	44	1	0	0	4	89	26605	1.2	6.5
	4	24	15.43	10.2	0.64292	0.25	82	2	0	0	4	8	26605	2.4	52.8
	5	25	16.10	10.4	0.64400	0.80	170	2	0	0	5	170	26605	0.8	170.3
	6	24	15.45	10.3	0.64375	1	106	2	0	0	6	128.5	26605	3.3	80.5
	7	24	15.54	10.9	0.64750	0.50	89	2	0	0	5	91	26605	1.2	28.1
	8	25	16.51	10.6	0.66040	1	99	2	0	0	7	144	26605	2.3	90.3

#### Table 5. Initial ship sailing information of voyage 2

	Day	Steaming hour (h)	Total fuel (tons)	Speed (knots)	Hourly fuel consumption (tons/h)	Bad weather ratio	Relative sea swell direction (degree)	Sea swell height (m)	Sea current type	Sea current value	Wind force (Beaufort force number)	Relative wind direction (degree)	Total cargo weight (MT)	Combined Wind Waves and Swell Height (m)	Relative Wind Wave Direction (degree)
535	1	24	14.45	11.2	0.60208	0	113	1	-1	0.6	3	90.5	31948	1.9	93.0
	2	24	14.41	10.8	0.60042	0	87	1	-1	0.6	4	154.5	31948	2.0	76.9
	3	24	14.35	9.2	0.59792	0.75	132	2	-1	1	6	177	31948	1.9	106.4
	4	24	14.36	8.9	0.59833	1	177	2	-1	1.5	6	160.5	31948	1.6	121.6
	5	24	14.33	9.7	0.59708	0.17	95	2	-1	1.5	4	117.5	31948	1.5	111.8
	6	24	14.36	10.5	0.59833	0	100	2	-1	1	4	100	31948	1.8	104.6
	7	24	14.45	11.5	0.60208	0.04	145	1	0	0	5	100	31948	2.3	106.1
	8	24	14.21	9.3	0.59208	1	145	2	-1	1.5	6	100	31948	3.0	113.0

536

We use the total 226 data entries (i.e., all the data entries in the entire dataset except 537 for the 16 records used to validate the optimization model) to construct the RF regressor. 538 Due to the lack of extreme valued data, predicting fuel consumption under too large or 539 too small speed values is highly likely to suffer from inaccuracy (Freidman et al., 2001). 540 Thus, we make predictions on fuel consumption with speed values ranging between 10% 541 and 90% from small to large in the training set, i.e., we exclude the 10% smallest and 542 10% largest speed values. The selected speed values are from 8.9 to 13.3 knots. The 543 fuel consumption prediction results are presented in Figure 4. For the 16 validation 544 records, we only have the real output value under the given speed. The performance of 545 the RF regressor on predicting the fuel consumption under the given speed of the 16 546 records are given in Table 6. It can be seen that the predicted fuel consumption under 547 the given speed is higher than the real fuel consumption.

548

549

550



532

551	(a) Prediction results of voyage 1	(b) Prediction results of voyage 2
552	Figure 4. Fuel consumption pro-	ediction results of the voyages
553		
554	Table 6. RF regressor perfo	ormance on predicting fuel
555	consumption of	the two voyages

Path NO	Real total fuel consumption	Predicted total fuel consumption	MSE	RMSE	MAE	MAPE
1	126.36	129.6335	0.5186	0.7201	0.6285	4.00%
2	114.92	116.6830	1.5702	1.2531	0.8950	6.24%

561

557 Apart from predicting fuel consumption under different speed values in each 558 segment, the RF regressor is also able to illustrate the feature importance of the input 559 variables when predicting fuel consumption. The feature importance generated by the 560 230 data entries is shown in Figure 5.



563

#### Figure 5. Relative importance of the input features

Figure 5 indicates that ship sailing speed is the most significant influencing factor on ship fuel consumption, which allies with most of the current literature. Total cargo weight also has a great influence on fuel consumption. Regarding sea and weather conditions, combined wind wave and swell height, relative sea swell, and relative wind wave direction can have more impact, while sea current type has the least impact on ship fuel consumption.

## 570 6.2 Validation of speed optimization model

We validate the performance of the proposed mathematical model by adopting CPLEX optimizer to find the optimal sailing speed in each segment which can minimize the total fuel consumption. A laptop (Intel Core i7, 2.20GHz, Memory 16.0G) is used to conduct the experiment with the programming language C++. The selected sailing

- 575 speed, sailing time, and fuel consumption in each segment of the two voyages are
- 576 shown in Table 7 and Table 8.

578

#### Table 7. Ship sailing information in voyage 1 after optimization

Day	Sailing	Sailing	Hourly fuel	Total fuel
	hours (h)	speed	consumption	consumptions (tons)
		(knots)	(tons/h)	
1	18.0451	13.3	0.812160	14.6555
2	17.8647	13.3	0.814638	14.5532
3	25.7895	9.5	0.569093	14.6766
4	22.4587	10.9	0.648483	14.5641
5	22.6087	11.5	0.684186	15.4685
6	18.5865	13.3	0.798043	14.8328
7	21.6198	12.1	0.758690	16.4027
8	19.9248	13.3	0.803543	16.0104
Total	166.898	/	/	121.1638
				(-4.11%)

579

580

Table 8. Ship sailing information in voyage 2 after optimization

Day	Sailing	Sailing	Hourly fuel	Total fuel
	hours (h)	speed	consumption	consumptions (tons)
		(knots)	(tons/h)	
1	28.2947	9.5	0.510766	14.4520
2	22.5391	11.5	0.666378	15.0196
3	16.6015	13.3	0.825215	13.6998
4	18.5739	11.5	0.706721	13.1266
5	24.5053	9.5	0.550893	13.4998
6	26.5263	9.5	0.545664	14.4745
7	24	11.5	0.689559	16.5494
8	23.4947	9.5	0.491945	11.5581
Total	184.536	/	/	112.380
				(-2.21%)

581

It takes only 0.05 and 0.03 second respectively to find the optimal solutions for 582 case 1 and case 2. After speed optimization, the dry bulk ship consumes 121.1638 tons 583 of fuel to complete voyage 1 and 112.38 tons of fuel to complete voyage 2 while 584 guaranteeing the arrival time to the destination. Compared with the real fuel 585 consumption of 126.36 and 114.92 tons in voyage 1 and 2, the ship can save 4.11% and 586 2.21% of total fuel consumption after speed optimization. It should be noted that the 587 predicted fuel consumption is a little higher than the real fuel consumption. If we 588 compare the fuel consumption after speed optimization and the predicted total fuel 589 consumption in these two voyages (i.e. 129.6335 and 116.6830), we can conclude that 590 6.53% and 3.69% of fuel consumption can be reduced, respectively. We can then 591 conclude that the two-stage fuel consumption prediction and speed optimization model 592 can help the bulk carrier ship to save 2% to 7% fuel to complete an 8-day voyage. Note 593 that as the data for training the RF regressor is limited and there can be inaccuracy in 594 fuel consumption prediction, the savings in fuel consumption may have variations.

595

#### 596 7. Extension and future research

597 Although numerous studies on ship fuel management are conducted based on ship 598 noon report, the data of ship sailing information and sea and weather conditions 599 provided by the noon report is actually limited (as discussed in Section 3.1) and the 600 time resolution is low: usually only one record for 24 hours. In order to make precise 601 fuel consumption prediction, which is the foundation of efficient ship fuel management, 602 one possible way is to incorporate more data features from other data sources, such as 603 sea and weather data from weather forecast website. For example, water depth can be 604 included for considering the influence of shallow water on fuel consumption. Besides, 605 temperature and salinity of water can also have an effect. Another possible way is to 606 combine noon report with ship sensory data, which can provide more ship sailing 607 features such as trim and draft condition with much lower time interval. Combining 608 sensory data can also help to develop sailing speed optimization model. If more data 609 can be obtained for a day, the division of sailing segment can be more flexible, e.g., by 610 the length of a fixed time such as 3h, 6h, or 12h voyage at the calm water set speed. In 611 addition, if more ship sailing information is accessible, it is easier to combine sea and 612 weather data with ship sailing data. In the current noon report, the sailing distance of 613 one day is usually more than 200 nm. As only one record is generated for each day, the 614 sea and weather conditions are viewed as identical in the whole sailing distance covered 615 by a whole day. However, sea and weather data can usually have a given resolution. For 616 example, if the resolution of sea and weather forecasting data is 0.5°, the associated arc 617 length is 30 nm. In addition, the weather forecast usually renews every few hours. For 618 example, the weather forecast provided by ECMWF renews every 6 hours. If we can 619 have 4-6 reports each day, the ship sailing data and sea and weather data can be 620 combined. Therefore, accurate and practical fuel consumption prediction model and 621 sailing speed optimization model can be proposed.

622

#### 623 8. Conclusion

624 Shipping companies are developing stronger motivations to improve ship fuel 625 energy efficiency for the purpose of complying with environmental conventions and 626 increasing their profits. This study proposes a two-stage fuel consumption prediction 627 and reduction model for a dry bulk ship to improve its energy efficiency based on the 628 noon report data. More specifically, at the first stage, a random forest regression model 629 is developed to predict the dry bulk ship's fuel consumption under different total carried 630 cargo, sea, and weather conditions. It is also validated that the proposed RF regressor 631 outperforms the widely used machine learning models such as ANN, SVR, and LASSO 632 for ship fuel consumption prediction. At the second stage, a speed optimization model 633 is proposed based on the fuel consumption prediction results at the first stage. The 634 objective of the optimization model is to minimize the total fuel consumption of the dry

635 bulk ship over a voyage which contains several segments by deciding the sailing speed 636 in each segment. The model is a mixed integer programming model which can be 637 efficiently solved by CPLEX. In the computational experiments, we use two 8-day 638 sailing voyage reports to test the performance of the two-stage model. The results show 639 that the proposed model can save fuel consumption to 2%–7% compared with the real 640 situation, which can also lead to significant CO<sub>2</sub> emissions reduction. In addition, the 641 influence degree of the input features on the total fuel consumption is also generated. 642 Similar to other related studies, it is indicated that ship sailing speed is the dominant 643 factor of ship fuel consumption, then followed by total carried cargo. Regarding sea 644 and weather conditions, combined wind wave and swell height, relative sea swell and 645 wind wave directions can also have remarkable impact, while the current type has the 646 least influence on ship fuel consumption. This paper considers the relationship between 647 ship sailing speed and fuel consumption rate in a non-analytical form, which improves 648 the common understanding about fuel consumption management. The proposed model 649 is one of the pioneering models which combine a machine learning model with an 650 optimization model in ship fuel consumption prediction and reduction. Based on the 651 model, shipping companies are able to finer plan the daily sailing speed of their ships 652 in order to reduce fuel consumption and CO<sub>2</sub> emissions.

653

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# Appendix A. Construction of decision tree regressor (Friedman et al., 2001; Harrington, 2012; Breiman, 2017)

870 The input information for decision tree construction contains the training set and 871 termination conditions. We denote the set of J input features as  $(x_1, x_2, ..., x_J)$ . An input 872 feature is denoted by  $x_j$ , and the value range of this J – feature is  $[x_j^{\min}, x_j^{\max}]$ . A 873 specific value of this feature is denoted by  $s_j$ ,  $s_i \in [x_j^{\min}, x_j^{\max}]$ . In addition, we denote 874 the training set containing N data entries as  $D = \{(x^1, y^1), (x^2, y^2), ..., (x^N, y^N)\}$ . A data 875 entry is denoted by  $(x^e, y^e)$  with e=1,...,N, where  $x_e = (x^{e1}, x^{e2},..., x^{ej},..., x^{eJ})$  is a 876 dimensional vector containing J features and  $y^e$  is a one dimensional output value. 877 The construction process of a regression decision tree based on CART algorithm 878 requires finding the *best split* pair  $(j^*, s_{j^*}), s_{j^*} \in [x_{j^*}^{\min}, x_{j^*}^{\max}]$  of the nodes when splitting. 879 Denote termination condition (a) to (c) as  $T_a$ ,  $T_b$ , and  $T_c$ . The main steps to construct 880 a CART decision tree are presented as follows:

Procedure 1: Construction of CART decision tree

Input	Training set $D$ and termination conditions $T_a$ , $T_b$ , and $T_c$ .
Output	Regression tree $f^{DT}(x)$ .
Step 1	Find the <i>best split</i> pair $(j^*, s_{j^*})$ of the current splitting node by solving the

following formula:

$$(j^{*}, s_{j}) \in \underset{j \in \{x_{i}, \dots, x_{j}\}}{\operatorname{arg min}} \sum_{e \in R_{ui}(j, s_{j}) \atop s_{j} \in \{x_{m}, \frac{1}{x_{j}}\}} (y^{e} - \frac{1}{|R_{m1}(j, s_{j})|} \sum_{e_{i} \in R_{ui}(j, s_{j})} y^{e})^{2} + \sum_{e \in R_{ui}(j, s_{j})} (y^{e} - \frac{1}{|R_{m2}(j, s_{j})|} \sum_{e_{i} \in R_{ui}(j, s_{j})} y^{e^{2}})^{2}],$$

where  $R_{m1}(j,s_j) = \{e = 1,...,N \mid x^{e_j} \le s_j\}$  and  $R_{m2}(j,s_j) = \{e = 1,...,N \mid x^{e_j} > s_j\}$ .

Step 2 Use the best split  $(j^*, s_{j^*})$  to split the current node into two nodes that contain

two sub datasets 
$$R_{m1}(j^*, s_{j^*}) = \{e = 1, ..., N \mid x^{ej} \le s_{j^*}\}$$
 and  
 $R_{m2}(j^*, s_{j^*}) = \{n = 1, ..., N \mid x^{ej} > s_{j^*}\}$  with output values as

$$c_{1} = \frac{1}{|R_{m1}(j^{*}, s_{j^{*}})|} \sum_{e_{1} \in R_{m1}(j^{*}, s_{j^{*}})} y^{e_{1}} \text{ and } c_{2} = \frac{1}{|R_{m2}(j^{*}, s_{j^{*}})|} \sum_{e_{2} \in R_{m2}(j^{*}, s_{j^{*}})} y^{e_{2}} \text{ , respectively.}$$

- Step 3 Repeat step 1 and step 2 in a depth-first manner until coming to a node that reaches one of the preset termination conditions. Then, this node becomes a leaf node and a new node for splitting is found by backtracking.
- Step 4 Repeat Step 3 until there is no more nodes that can be split. Finally, the total training set is separated into M mutually exclusive sub-sets  $R_1, R_2, ..., R_M$ , and a sub-set is denoted by  $R_m$ . The decision tree model can be presented by

$$f^{DT}(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$$
, where  $I(x \in R_m) = \begin{cases} 1, x \in R_m \\ 0, x \notin R_m \end{cases}$ 

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