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In-cylinder pressure prediction for marine engines using machine learning

Chaitanya Patil[1], Gerasimos Theotokatos[1], Konstantinos Milioulis[2]
[1]Maritime Safety Research Centre, Department of Naval Architecture Ocean and Marine Engineering,
University of Strathclyde, Glasgow G4 0LZ, UK
[2]Datum Electronics, UK

First principle Digital Twins (DT) for marine engines are widely used to estimate in-cylinder pressure, which is a key parameter informing health of ship power plants. However, development and application of DT faces barriers, as they require exhaustive calibration and high computational power, which render their implementation for shipboard systems challenging. This study aims at developing a data-driven DT of low computational cost for predicting instantaneous pressure. Two different approaches using Artificial Neural Networks (ANN) with distinct input parameters are assessed. The first predicts in-cylinder pressure as a function of the phase angle, whereas the second predicts the discrete Fourier coefficients (FC) corresponding to the in-cylinder pressure variations. The case study of a conventional medium speed four-stroke diesel marine engine is employed, for which the first principle DT based on a thermodynamic, zero-dimensional approach was setup and calibrated against shop trials measurements. The DT is subsequently employed to generate data for training and validating developed ANNs. The derived results demonstrate that the second approach exhibits mean square errors within $\pm 2\%$ and requires the lowest computations cost, rendering it appropriate for marine engines DTs. Sensitivity analysis results verify the amount of training data and number of Fourier coefficients required to achieve adequate accuracy.

KEYWORDS

Marine engines, Data-driven DT, Machine learning, Artificial Neural Networks, Fourier Series

ABBREVIATIONS

DT: Digital Twin
CAD: Crank Angle Degrees
ANN: Artificial Neural Network
0D-3D: Zero Dimensional-3 Dimensional
CBM: Condition Based Maintenance
RMSE: Root Mean Square Error
MSE: Mean Square Error
R^2: Coefficient of determination

INTRODUCTION

Maritime transportation accounts for around 80% of the world freight movements, considerably impacting the environment. Several technologies and strategies are developed to maintain maritime transport machinery including marine engines, power plants with a support from first principles digital twins (DT), which are based on thermodynamic and fluid dynamic principles and pertinent conservation laws. These thermodynamic DT are proven effective for predicting performance parameters of thermal engines. However, these DTs are required to solve differential equations depending on dimensionality of the problem from 0D to 3D. These type of calculations demand considerable computational power and cost rendering their shipboard application challenging. Hence, the ship operators are reluctant to implement them for shipboard use. A fast and accurate solution to predict the marine engines performance is more suitable for shipboard applications.

The in-cylinder pressure is a key parameter representing the combustion phenomena inside cylinders of marine engines and provide information for fault detection, diagnosis and prognosis as reported in Tsitsilonis and Theotokatos [2018, 2021]. Hence, prediction of instantaneous in-cylinder pressure is crucial for health analysis of marine engines. Digital twins are widely used tools to predict the combustion and eventually the engine in-cylinder pressure variation. They are very common in several industrial sectors like automotive, marine, and energy . Apart from DT, efforts are made to develop a concept of a dimensionless pressure curve in the frequency domain rendering prediction of in-cylinder pressure estimation as important aspect to ensure proper functioning of reciprocating combustion engines Zeng and Assanis [2004]

Artificial Neural Networks (ANN) are data-driven based approaches that can be used to predict the performance parameters of mechanical systems. Nowadays, ANNs are getting popular in the shipping industry. Review of applications of ANN in internal combustion engines is reported by Bhatt and Shrivastava [2022]. The effectiveness of ANNs is proved for applications requiring the prediction of marine diesel engine performance Noor et al. [2016], Non-linear Auto Regressive Exogenous input (NARX-ANN) Raptodimos and Lazakis [2020] and Fuel oil consumption prediction

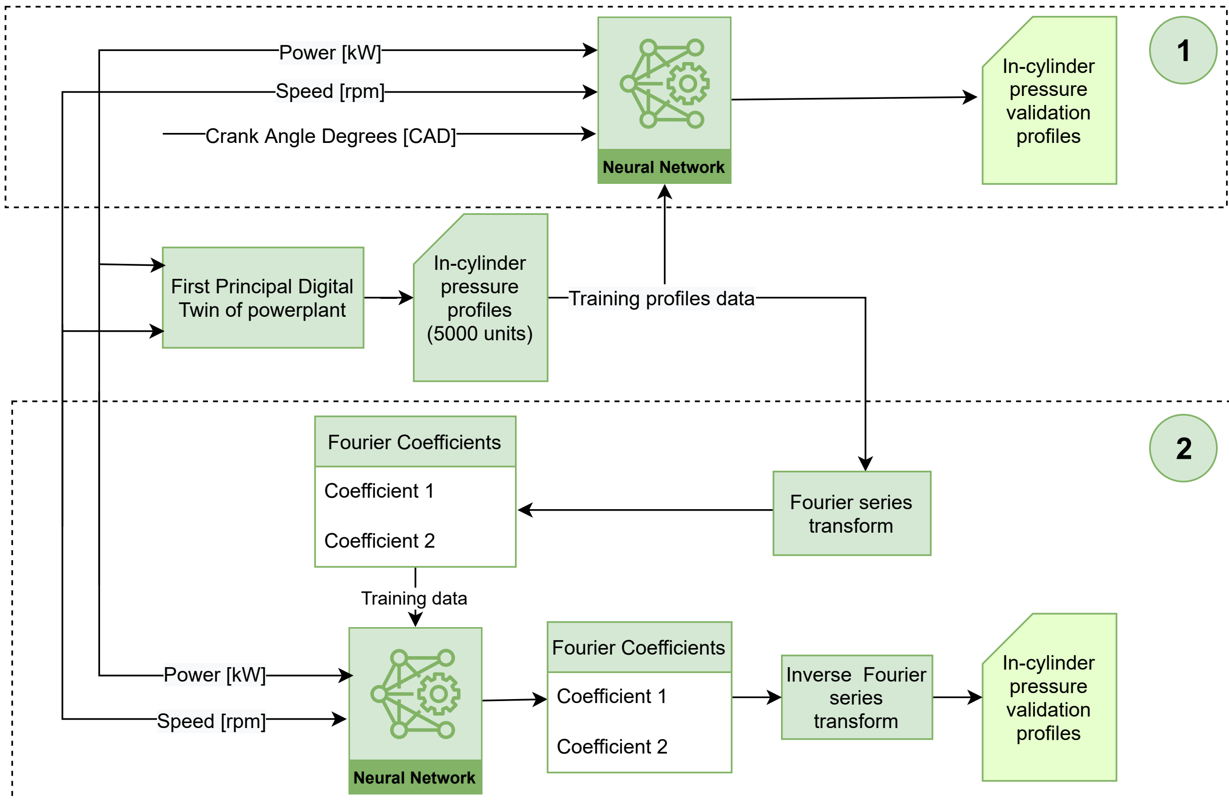


Figure 1: Methodology of the study depicting two approaches (highlighted by 1 and 2) used to form the data-driven DT.

from ship main engine Gkerekos et al. [2019]. Apart from performance prediction, ANNs are utilised to carry out condition based maintenance (CBM) for fishing vessels with medium speed diesel engines Basurko and Uriondo [2015] and marine propulsion system Cipollini et al. [2018]. Moreover, ANNs are useful for fault diagnosis in ship systems including the diagnosis of clearance in valves of engines Zhu [2009], faults in engine cooling system Zhou and Xu [2010] and bearing faults Yang et al. [2007]. They are also utilised to detect the abnormalities in the system in absence of any fault with a data collection Raza and Liyanage [2009]. In general, health assessment and condition monitoring of the ship machinery systems can be improved by ANN with self organising maps for engine Raptodimos and Lazakis [2018], multi net neural networks system with non intrusive sensors Porteiro et al. [2011] and convolutional neural networks Wang et al. [2021].

The literature review points out methods and gaps to determine the engine in-cylinder pressure. DT require exhaustive calibration, high computational power, and advanced processors, rendering. On the other hand, data-driven models based on machine learning techniques are utilised only to estimate quasi-steady operating parameters as time series, however lacking the ability to predict instantaneous signals. Some networks based on complex radial basis functions (RBF) are studied using the vibrations and speed signals to estimate the pressure profile from combustion engine by Johnsson [2006]. However, their increased complexity with RBF and extra sensors requirement hinder the direct application of these networks for ships machinery applications.

This study aims at developing a data-driven DT of low computational cost to predict the in-cylinder pressure at healthy conditions of a case marine engine using the minimum set of input parameters. The required training data is generated through the use of a thermodynamic DT, which was setup for the case study of a marine four-stroke engine. This DT was validated against in-cylinder pressure signals experimentally measured in five operating points. Two approaches for developing data-driven DT based on ANN are considered and compared based on the root mean square errors obtained using estimated values and baseline values (in-cylinder values from DT). The comparison is done over the full operating envelope of the case marine engine. A sensitivity study is performed on the second ANN DT to assess the impact of the training data amount and the harmonic orders (*Fourier series coefficients* number) on the DT prediction accuracy.

METHODOLOGY

The detailed methodology is described in this section consisting following steps:

- Step I: Data generation
  In-cylinder pressure profiles for all the steady operating points,

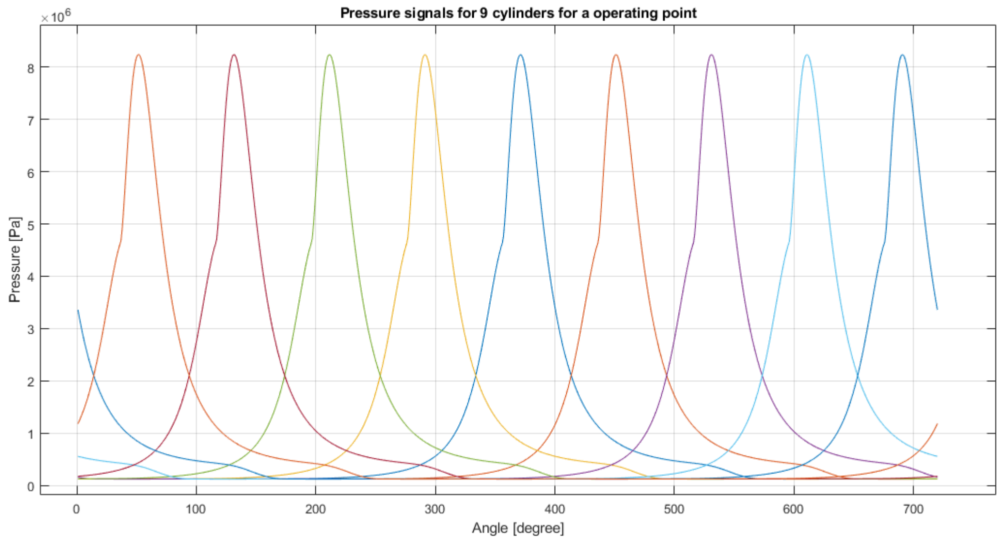


Figure 2: In-cylinder pressure profiles obtained by calibrated DT referring to an operating point of the considered marine engine.

covering working envelope of marine engine, are generated using the developed zero-dimensional DT.

- Step II: DT Development
  An Artificial Neural Network is developed and trained using data generated from previous step. Two approaches are used to form ANNs as showcased in schematic of methodology (Figure 1). The first approach develops an ANN by considering as input the engine speed, power, cylinder number and crank angle, whereas it provides as output the in-cylinder pressure. The second approach develops another ANN to predict the Fourier coefficients representing a pressure curve using as input the engine speed, power and cylinder number. The in-cylinder pressure for each operating point is reconstructed based on these coefficients.

The data pre-processing required for DT development in step II is described in Subsection DT development. It involves, the pressure profile conversion required for second approach (Subsection Definition of pressure profile using Fourier transform), feature selection (Subsection Feature selection), splitting data into training and testing data sets (Subsection Training and validation) and data standardisation(Subsection Feature standardisation).

Step I: Data generation

Initially, a thermodynamic digital twin (based on thermodynamic principles and conservation laws) is setup and calibrated to match the engine performance parameters according the shop trials. The marine engine used in this case is medium speed, 9 cylinder, 4-stroke, turbocharged engine from Wärtsilä. The information related to the reference engine is presented in Table 1. The MATLAB platform is used to develop the 0D DT of each subsystem. The detailed information about the DT can be found in Tsitsilonis et al. [2021], Tsitsilonis and Theotokatos [2021]. The framework developed by

MCR	9,450 kW @ 500 RPM
No. of Cylinders	9
Cylinder Bore	460 mm
Clutch-in Speed	300 RPM
Turbocharger	ABB TPL 77-A30

Table 1: Reference system technical specifications.

Tsitsilonis and Theotokatos [2022] is used to calibrate the engine. The calibration involves the determination of the combustion and friction mean effective pressure parameters for the reference operating point. Subsequently, the calibration determines the values of the Woschni-Anisits combusiton model constants by considering all the remaining shop test operating points. The DT is validated as per the engine shop tests results. The validation results can be found in Tsitsilonis and Theotokatos [2022]. The DT is further used to generate series of data points (in-cylinder pressure profiles) considering the engine operating envelope. Figure 2 presents the derive in-cylinder pressure profiles obtained by the calibrated DT. Around 5000 operating points spread all over the operating envelope of the considered marine engine are simulated ranging from 350 to 500 rpm.

Step II: DT development

This section focuses on development of DT based on ANN to predict in-cylinder pressure. Two approaches mentioned in previous sections are used to form a machine learning problem based on feature selection process.

Feature selection

Feature selection is an important step to select the required input parameters fro the DT development. They should contain the required information to predict the target variable (in-cylinder pressure in this case). The engine speed and power are the important parameters to represent an engine operating point. However, the target variable is an instantaneous function of the crank angle (0–720 degrees for four-stroke engines). Therefore, two approaches are considered herein. The first one follows the traditional instantaneous problem formulation with the crank angle as input along with engine performance parameters like engine speed and power to predict pressure at respective crank angle. While, the second approach accepts only engine performance parameters to predict complete in-cylinder pressure curve for 720 crank angles. The first approach (Number 1 in Figure 1) considers the estimation of the in-cylinder pressure mapped as a function of the engine speed, power, cylinder number and crank angle, according to the following equation:

$$P(\alpha) = f(N, P, n_{cyl}, \alpha) \tag{1}$$

where N, P, n_{cyl} are the engine speed, power and cylinder number respectively, whereas α denotes the crank angle.

The second novel approach (Number 2 in Figure 1) considers only the engine speed and power as input to derive the in-cylinder pressure diagram (complete engine cycle) at the considered operating point. However, an extra step is inserted for converting the in-cylinder pressure signal to a set of discrete *Fourier coefficients* considering a specified number of harmonic orders (N). The in-cylinder pressure signal is approximated and mapped as function of engine speed and power according to the following equation:

$$P(\alpha) = f(C_1, C_2..C_N) = f(N, P) \tag{2}$$

The method of converting in-cylinder pressure curve to *Fourier series coefficients* is based on the use of *Fourier Transform* as mentioned in following subsection. These Fourier coefficient are employed as the target variables for neural network and subsequently used to reconstruct the finally predicted in-cylinder pressure signal.

Definition of pressure profile using Fourier Coefficients

The characteristic in-cylinder pressure curve contains crucial information related to the efficiency, power, and emissions from internal combustion engines. The pressure measurement is carried out from each cylinder of a marine engine as a function of crank angle degrees associated to particular operating points. However, it is easier to use pressure signals as a function of discrete coefficients rather than crank angular measurement by reducing the number of dimensions of machine learning problem. In the open literature, a number of studies are reported, with the aim to reconstruct in-cylinder pressure pulse curve using Fourier coefficients for several applications by Johnsson [2006], Zeng and Assanis [2004], Taraza et al. [2005]. Similar strategy is used to convert simulated pressure curves from Section Data generation as a function of coefficients called *Fourier Coefficients* as follows,

$$p(\alpha) \Rightarrow f(FC1, FC2, ...) \tag{3}$$

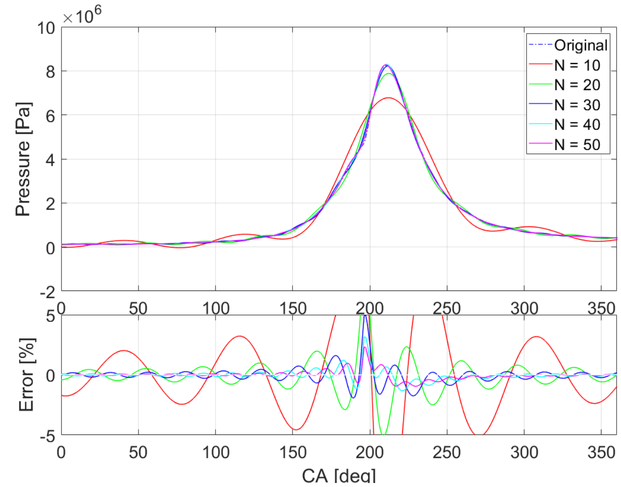


Figure 3: Reconstruction of pressure signal from N harmonic orders with 2N+1 number of *Fourier coefficients* (x-axis is crank angle degrees (CAD)).

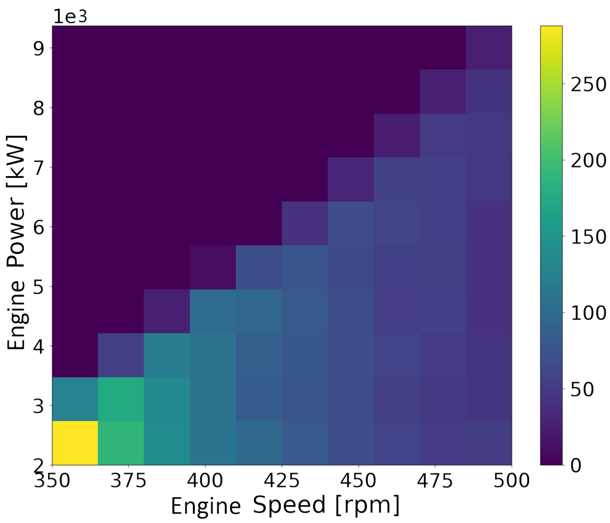
The Fourier analysis can be used to convert the periodic function (pressure) repeating for every two revolutions (for four-stroke engine) into Fourier series using the following equation, as reported in Zeng and Assanis [2004],

$$p(\alpha) = \mathrm{a}_0 + \sum_{n=1}^{\infty} \mathrm{a}_n cos\left(\frac{2\pi n\alpha}{T}\right) + \sum_{n=1}^{\infty} \mathrm{b}_n sin\left(\frac{2\pi n\alpha}{T}\right) \tag{4}$$

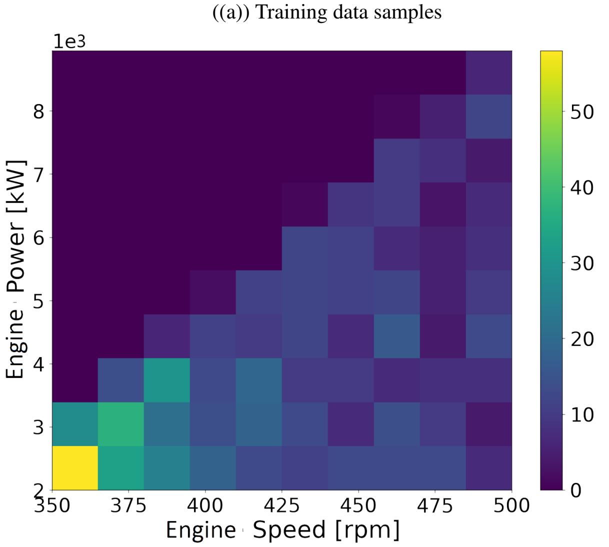
Where,

$$\begin{aligned} \mathrm{A}_0 &= \frac{1}{T}\int_{-T}^{+T} p(\alpha)d\alpha \\ \mathrm{A}_n &= \frac{1}{T}\int_{-T}^{+T} p(\alpha)cos\left(\frac{2\pi n\alpha}{T}\right)d\alpha \\ \mathrm{B}_n &= \frac{1}{T}\int_{-T}^{+T} p(\alpha)sin\left(\frac{2\pi n\alpha}{T}\right)d\alpha \end{aligned} \tag{5}$$

The coefficient A_0 is the average value of the in-cylinder pressure within the engine cycle, whilst A_N and B_N coefficients represent the multiplication factors (amplitudes) to the *cosine* and *sine* functions with N harmonic orders. The number of harmonic orders required to exactly recreate the pressure curve (with practically zero error), depends on the pressure signal sampling number (typically 1^oCA sampling requires 720 harmonic orders for four-stroke engine). However, referring to the goal of reducing dimensions for machine learning problems, less number of harmonic orders should be selected without loosing meaningful information for estimating faults. Figure 3 represents the reconstruction of the in-cylinder pressure profile using 2N+1 number of Fourier coefficients. As N increases, the error in comparison with actual in-cylinder signal reduces. Therefore, N=50 (101 Fourier coefficients) is selected for comparison of two approaches proposed in this study. A sensitivity analysis based on the N to identify the DT error is presented in the results section.



((a)) Training data samples



((b)) Test/Validation data samples

Figure 4: Histogram of samples used for training and validation/test data over the operating range of the investigated marine engine (test/train ratio = 0.15)

Feature standardisation

The data used to create ANN needs pre-processing to ensure better accuracy. Standardisation of data (also called as Centering) is done to set mean of each input/output parameter equal to zero. This captures only the variation in the data points to determine hyper parameters is ANN.

All numerical attributes in the data set are standardised by removing the mean and scaling to unit variance. For a numerical attribute x, a standardised attribute x' is produced by,

$$x' = \frac{x - \mu}{\sigma} \tag{6}$$

where μ is the mean value the attribute, and σ is the standard deviation. All attributes are standardised, so that they can contribute equally to the objective function that is used for training of developed DT.

Training and validation data

After standardisation, the generated data is classified into training and validation/test data sets. Training data is normally used for selecting the hyper parameters/weights of the ANN based on back propagation of error discussed in the next section. Validation/test data is kept separate from the training process. This test data is used after to test the DT and validate the accuracy.

The selection of this tests data is critical to check the DT accuracy over the engine operating envelope. The test/train ratio (γ) determines the percentage of data used for this separation, and is defined by the following equation:

$$\gamma_{Test/Train} = \frac{N_{Test}}{N_{Train}} \tag{7}$$

This study employs testing samples for validation of accuracy of DT, following the training process. In this respect, the distribution of test samples should be similar to training data sets including data points all over the operating range. Figure 4 presents the distribution of training and validation data-sets for the considered marine engine operating envelope.

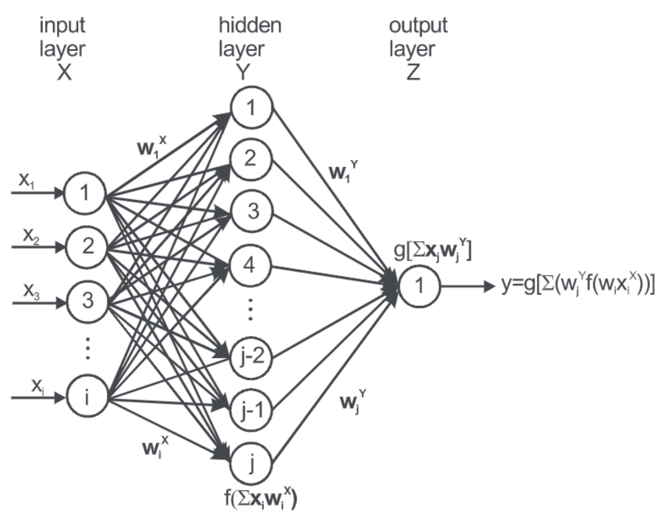


Figure 5: Artificial Neural Network (Multi Layer Perceptron) with one hidden layer Szoplik [2015].

Artificial Neural Networks (ANN)

Artificial Neural Networks (ANN) are inspired by biological nervous systems. They are used to perform machine learning tasks including classification and regression. ANNs are extremely versatile as they can accurately model complex non-linear behaviour of any system based on the data provided.

MultiLayer Perceptron (MLP) networks, which are also known as multilayer feed forward networks, are widely used in practical applications. A typical multi layer feed forward network is represented in Figure 5. Two important parameters of MLP are the number of hidden layers (between input and output) and the number of units per layer (hidden layer sizes). Excluding the input and output layers, different architectures call for different number of hidden layers.

The number of neurons in the hidden layer is also not specified in literature, and thus they must be selected by trial and error basis. This study considers two approaches employing ANN to predict the in-cylinder pressure and compare the results. Therefore, the same number of hidden layers and neurons is selected for both approaches. Considering the non-linear relationship between inputs and output, an activation function called Exponential Linear Unit (ELU) is used at each neuron of hidden layer followed by a linear activation function at the output layer.

Table 2: Summary of the first modelling approach

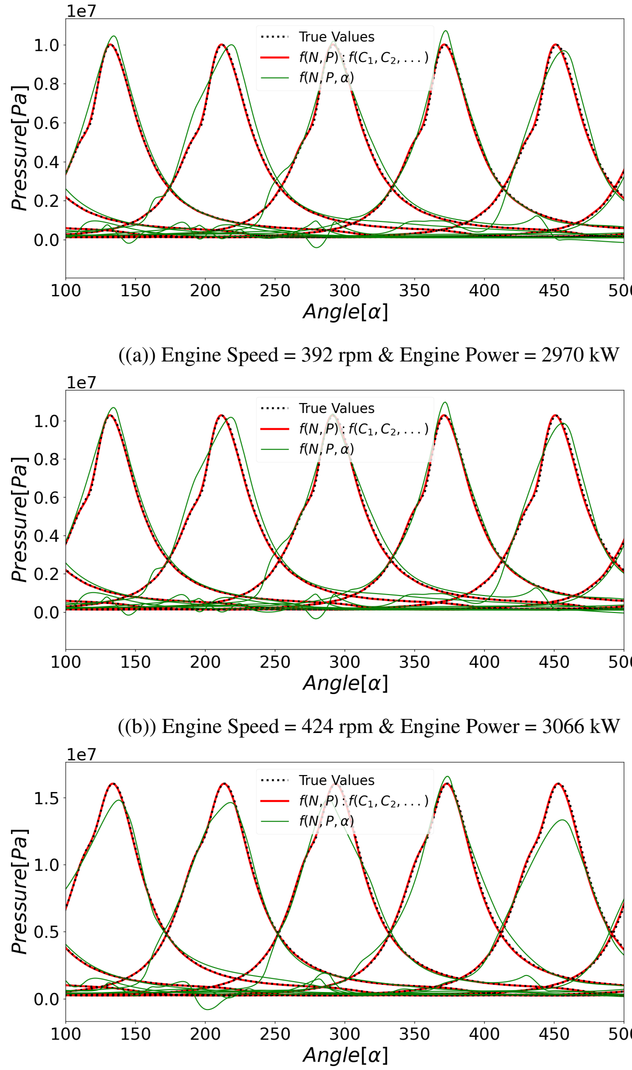
Layer (type)	**Output shape**	**Parameters**
Input layer	(None,4)	0
Hidden layer (Dense)	(None,10)	50
Hidden Layer (Dense)	(None,10)	110
Output layer	(None,1)	11

The details of the developed ANNs based on the first modelling approach is provided in Table 2. The input layer consists of 4 input parameters, in specific, engine speed, engine power, crank angle (α) and cylinder number, based on which the in-cylinder pressure is predicted. The output layer has only one parameter, which is in-cylinder pressure at given crank angle (α). The second approach employs only 3 inputs (engine speed, power and cylinder number) and estimated in total 909 outputs (101 per cylinder) with A_N, B_N and A_0 corresponding to 50 harmonic orders (N=50). The in-cylinder pressure for each cylinder is then calculated based on these 101 (909 for 9 cylinders) coefficients. The details of this ANN structure are provided in Table 3.

Table 3: Summary of the second modelling approach

Layer (type)	**Output shape**	**Parameters**
Input layer	(None,3)	0
Hidden layer (Dense)	(None,10)	30
Hidden Layer (Dense)	(None,10)	110
Output layer	(None,909)	999

The training of the two ANNs is carried on the training data sets selected from Section . The *Adam* optimiser is used to reduce



((a)) Engine Speed = 392 rpm & Engine Power = 2970 kW

((b)) Engine Speed = 424 rpm & Engine Power = 3066 kW

((c)) Engine Speed = 492 rpm & Engine Power = 6116 kW

Figure 6: Performance comparison two approaches w.r.t. true (reference) values [$f(N, P, \alpha, n_{cyl})$ and $f(N, P, n_{cyl})$]

the Root Mean Square Error (RMSE) between the reference values y and predicted values $\hat{y}$ by using back propagation of gradients over hyper parameters determined in previous steps in optimisation process. *Adam* optimiser is able to adapt to new learning rates based on the number steps required to reach global minimum for RMSE. The RMSE is calculated using following equation:

$$RMSE = \sqrt{\sum_{i=1}^{n} (y - \hat{y})^2} \quad (8)$$

The accuracy of the given regression models is determined by the coefficient of determination (R^2) on the validation data, which is calculated by the following equation:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y-\hat{y})^2}{\sum_{i=1}^{n}(y-\bar{y})^2} \quad (9)$$

where $\sum_{i=1}^{n}(y-\hat{y})^2$ is the sum of residuals, and $\sum_{i=1}^{n}(y-\bar{y})^2$ is the total sum of squares (equal to variance) of the validation data with $\bar{y}$ denoting the mean value. In the best case, when the modelled values exactly match the reference values, R^2 becomes equal to 1.

RESULTS

Based on the followed methodology, the ANNs are trained on the training data selected from pool of synthetic data generated through simulations. The results from the training and validation of the two approaches are presented in this section. The accuracy or error mentioned in this section represents the test/validation data sets only.

The time taken to train the DT through the back propagation of error varies with the number of inputs and the data used for training. Therefore, to compare the two methods, apart from the structure of ANN, the number of selected harmonic orders (N) are kept constant to 50, whereas the test to train ratio (γ) is fixed to 0.15.

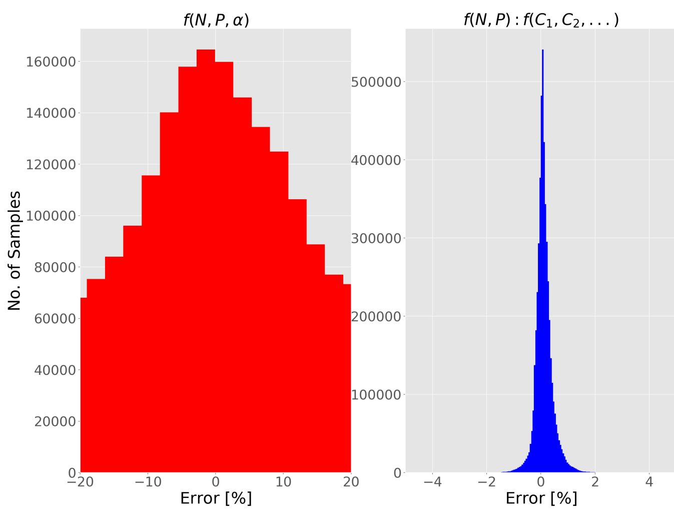


Figure 7: Histogram of error (in percentage) in estimation of in-cylinder pressure from the two approaches.

The training is performed in batches called Epochs. In machine learning, an epoch is a complete iteration over a data set during the training process. During each epoch, the DT processes the entire data set, making updates to its hyper parameters based on the optimisation algorithm used. Each epoch represents that all data is used by the DT during training with same test to train ratio. In total 200 epochs are used during training for both mentioned approaches. The training time (optimisation) of the first approach was 13 minutes per epoch on average. The second approach with N=50 takes only 45 seconds per epoch. Therefore, from the time perspective, the second approach exhibits faster training, even though the number of output nodes are higher.

Figure 6 presents the actual estimation of in cylinder pressure for 5 out of 9 cylinders for three operating points. The plots are zoomed to provide the performance of the two approaches in comparison with the respective reference values (dotted lines). The second proposed approach with *Fourier coefficients* pressure estimation provide better accuracy compared to the first approach predictions. The error histograms for the two approaches are presented in Figure 7. It is evident that the percentage error from the second approach (blue) has 95% of errors being between $\pm1\%$, whilst the single point based approach $f(N,P,\alpha)$ exhibits errors spread over wider range. Hence, from the accuracy point of view, the second approach demonstrates superiority.

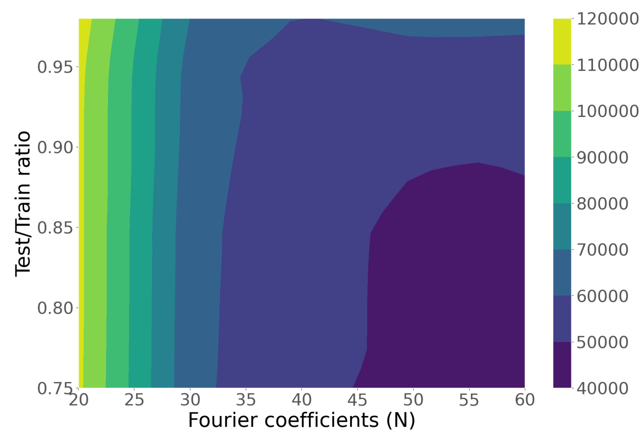


Figure 8: Sensitivity of RMSE [Pa] (high error with high brightness) with the test/train ratio and the harmonic orders number (N) used in the second ANN model for in-cylinder pressure estimation.

Following the comparison of these two approaches, the sensitivity study for the second approach is carried out to assess the change in RMSE with the harmonic order number and the amount of data used for training. Figure 8 showcases the contour plot of root mean square error with variation in N and test to train ratio used for training. It is evident that the harmonic orders number used to define the in-cylinder pressure curve greatly affects the error. For more than 45 harmonic orders, reasonable accuracy is exhibited. The test to train ratio has minimum effect on the error, even if the ratio is quiet higher than 0.75. Therefore, the DT can be trained with only 25% of the 5000 operating points randomly selected to achieve sufficient accuracy. This reduces the computational effort requited for the data generation by employing the physical DT (which is more computational expensive). The data-driven approach substantially reduces the required computational effort.

CONCLUSIONS

A cost effective data-driven DT was developed for estimating in-cylinder pressure of a marine engine based on two different approaches. The first approach uses the engine speed, power and crank angle to predict the single point pressure value at given crank angle degree. The second approach uses only the engine speed and power as input to predict the in-cylinder pressure diagram for the whole engine cycle. An extra step is introduced in second approach to convert the instantaneous pressure curve into discrete Fourier coefficients corresponding to a specific harmonic order number (N), reducing the dimensions and thus the required computation time. The main findings drawn from the comparison of the two approaches (using ANNs with same hidden layers and neurons) are as follows.

1. The required ANN training time for the second approach (with the harmonic order number N=50) was 94% less compared to the first approach, thus proving its applicability.

2. The second approach exhibited percentage errors (compared to reference values) in the range of $\pm 2\%$ for in-cylinder pressure prediction.

3. The sensitivity analysis revealed that, minimum 10% of data (1000 samples) can be used with the harmonic order number N=45 to achieve RMSE between 4000-5000 Pa. This corresponds to accuracy (R^2) close to 0.99%.

The second modelling approach proves that only 10% simulation data from thermodynamic DT can be used to train data-driven DT. The developed data-driven DT predictive ability is limited within the engine operating envelop that was used for training. Application of these data-driven DT further simplifies the diagnostics and prognostics of the marine power plants providing the engine in-cylinder pressure at healthy conditions.

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