Advances in Reliability, Safety and Security, Part 2 – Kołowrocki, Magryta-Mut (eds.)

Advances in Reliability, Safety and Security

ESREL 2024
Monograph Book Series

Two Phase Physics Informed Deep Learning Architecture For Remaining Useful Life Prediction

Aditya Sanju[a], Zhiguo Zeng[b,], Mihaela Mitici[c], Anne Barros[b], David Coit[d]

[a]*Department of Manufacturing Engineering and Industrial Management, College of Engineering, Pune, Pune, India*
[b,d]*Chair on Risk and Resilience of Complex Systems, Laboratoire Genie Industriel, Centralesupelec, Universite Paris-Saclay, France*
[c]*Faculty of Science, Utrecht University, Heidelberglaan 8, 3584 CS Utrecht, The Netherlands*
[e]*Department of Industrial and Systems Engineering, Rutgers University, 96 Frelinghuysen Road, Piscataway, NJ 08854, USA*

Abstract

Prognostics and Health Management (PHM) has proven to be an effective tool for reliability and safety of systems, especially with the rise of Industry 4.0. For PHM of systems, AI-based condition monitoring techniques have significantly improved the performance of remaining useful life (RUL) predictions. However, most RUL prediction models based on traditional deep learning do not consider physical-knowledge during their training process and have no physical constraints in the model dynamics. As a result, the model lacks explainability and generalizes poorly on unseen data. Physics-informed deep learning intends to address these concerns by embedding physical knowledge in training the deep learning models. In this paper, a two-phase physics-informed deep learning architecture is proposed to integrate physical knowledge for RUL prediction. In phase I, the monitored degradation data is filtered using a neural network trained on historical degradation data. When training the network, physical knowledge on the degradation path is embedded in the loss function. In phase II, the filtered degradation measurements are used to train a second neural network for predicting the RUL. The proposed architecture is illustrated on an open-source dataset of lithium prismatic batteries. The results show that considering the physical knowledge worsens the model's capability to fit the degradation path, but improves its performance for RUL prediction.

Keywords: prognostics and health management, remaining useful life, physics-informed machine learning, lithium battery

1. Introduction

With the rise of Industry 4.0, PHM has grown to be a necessity in order to intensify reliability and safety of systems. PHM aims to predict the failure of a system preemptively. Based on such predictions, informed planning decisions can be made, and unexpected downtime can be limited. This is mainly done by assessing the system dynamics and modeling the degradation process. By monitoring the degradation process, predictions of the remaining useful life (RUL) of a system are made using different methods.

Existing methods for degradation modeling and RUL prediction can be broadly classified into physics-based models and data-driven models (Bhat, 2023). Physics-based models capture the underlying governing physics of the system, and construct an empirical relationship between the variables. They make use of mathematical functions and equations to represent the degradation of the system. A thorough analysis of the system to uncover all the required precursors for the failure of the system, is a requisite for physics-based modeling. However, this is often difficult to achieve practice due to the complexity of the systems. Data-driven methods do not require a complex analysis of failure modes and an identification of all responsible precursors. In fact, these are black - box models that are trained based on observed data, and infer the model parameters from it (Zio, 2022; Jardine, 2006). Such data-driven models are capable of constructing relationships between system parameters directly from observation data. When the training data are sufficient, the data-driven models have proven to be powerful in modeling complex degradation behavior and predicting the RUL. However, the need to use large amounts of data to learn the failure and degradation behavior limits the application of data-driven models in practice. Additional drawbacks for data-driven models are issues related to overfitting and poor generalization as no physical knowledge on the degradation and/or failure processes is considered. To address these limitations, hybrid physics-informed machine learning models are proposed that leverage the physical knowledge together with data-driven models to model complex degradation behaviors. Physics-informed machine learning uses physical knowledge to

complement traditional machine learning models. In the literature, there are two common ways to inject physical knowledge into data-drive machine learning models (Xu, 2022):

i) Physics-informed loss function - This approach embeds physical constraints of the system into the loss function of the neural network. A typical physics-informed loss function is as follows:

$$Loss = Loss_{ML} + Loss_{Phy}$$

where the first term is the typical loss function used in training machine learning models, commonly defined as the absolute difference or the mean squared difference of the true and predicted value. The second term in the loss function enforces physical constraints into the system. Typical forms of the physical constraints include ordinary differential equations, partial differential equations, or other equations which describe the behavior of the system.

ii) Physics-informed architecture - This approach uses physics-based models and data-driven models separately, and then fuses the results from the two individual models. This is generally done by using the output of the physical model as an input to the data-driven model. The embedding of physical knowledge into the neurons or the layers of the neural network form a physics-informed architecture. Bayesian physics-informed models also fall under this category where the probabilistic nature is introduced in traditional machine learning models. The use of such hybrid approaches has been successful in developing robust, theory-affirming models. They also require less training data as the physical knowledge can help guide the model (Chao, 2022). These models have been powerful in generating a solution space for ordinary and partial differential equations (Raissi, 2019). In PHM, physics-informed machine learning models have been applied and proved to significantly improve the performance of RUL prediction (Y. He and Wang, 2022). In this paper, we develop a two-stage physics-informed neural network for RUL prediction of complex systems. In the first phase, we use physics to filter the data using a neural network thereby creating a noise filtered dataset. This allows for the neural network in the 2nd phase to make informed predictions about the RUL of the system. We illustrate our proposed approach for the RUL prediction of lithium prismatic batteries. The results show that our approach estimates the RUL of the batteries with decreasing prediction errors closer to the actual time-to-failure compared to the methods deprived of physical knowledge.

The rest of this paper is organized as follows. Section-I gives a brief overview of the existing techniques and discusses the challenges associated with fully data-driven methods for RUL prognostics. In Section-II, the architecture of a physics-informed neural network for RUL prognostics is given. Section-III provides an overview of the results obtained for a case-study on RUL prognostics for lithium prismatic batteries. Section-IV provides concluding remarks and future scope.

2. A two-stage physics-informed neural network architecture for RUL predictions

Machine learning methods have been widely used in the field of PHM for fault prognosis of systems. Unlike semi-supervised learning models like - Kalman filter (KF), Extended Kalman filter (EKF), Particle filter (PF) who follow a recursive approach, supervised learning models are trained on data without the need to recursively update the state variables. This paper proposes a physics-informed machine learning architecture which uses inferred physical knowledge to constrain the model's predictions. The developed RUL prediction framework comprises two phases, as shown in Fig 1. In phase 1, the acquired raw condition-monitoring data is filtered through a convolutional neural network. The purpose of this phase is to remove the noise in the condition-monitoring data so that the cleaned data can be used for training a neural network for RUL prediction in phase 2. Physical knowledge on the degradation path is embedded in the neural network (See Section II-A). After removing the noise, the cleaned condition-monitoring data are fed to phase 2, where a new neural network is trained for RUL prediction. Physical knowledge on the relationship between RUL and time can be encoded in this phase (see Section II-B).

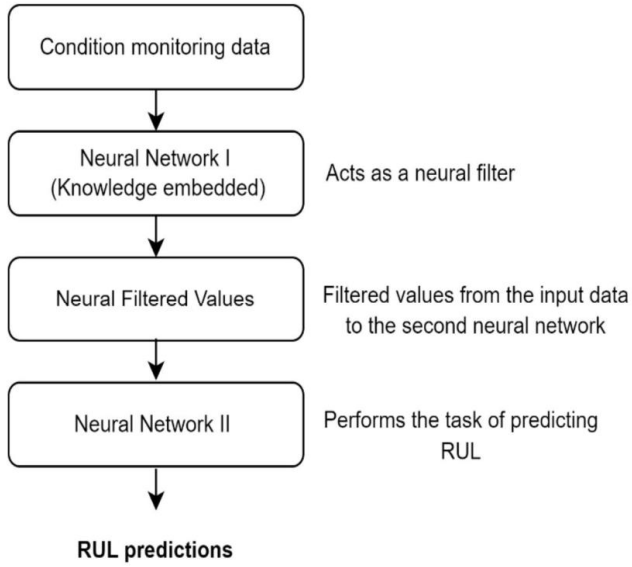


Fig. 1. Architecture of the 2-phase Neural Network for RUL prediction.

2.1. Neural Network - I

In phase 1, a neural network is designed to filter the noise in the original condition-monitoring data. These condition-monitoring data consists of variables that have a direct or an indirect effect on the degradation behavior. Since condition-monitoring data are acquired from sensors, these are usually subject to noise. As per Fig. 1, the condition-monitoring data is fed into the first neural network (NN-I), which primarily performs the task of filtering the noisy dataset using a knowledge-embedded loss function. Therefore, the output of the network is the same variable as the input variable, after removing the noise.

The neural network used for filtering comprises one LSTM layer (64), two dense layers (16 and 1 neurons, respectively), and multiple dropout layers. The LSTM uses a sliding window where the set of values used in the window are used to predict the next value. The sliding window uses a set of 32 data points of battery capacity values as an input to predict the next value of the battery capacity. The hidden dense layer adopted a piecewise linear function (ReLU) and the output layer adopted a linear activation function. The input and the output dimension is the same, i.e., (32,1). The network is then trained on a large number of historical degradation paths.

Physical knowledge on the form of degradation path can be integrated in the training of the neural network. In this paper, we propose to integrate the physical knowledge into the loss functions used in the training phase, as shown in Eq. (1).

$$Loss = |y_{true} - y_{pred}| + |y_{pred} - y_{theoretical}| \quad (1)$$

The first modulus term in Eq. (1) is the mean absolute error between the true and predicted value. The second modulus term is the physics-informed error and describes our understanding about the physical knowledge on the degradation path, where $y_{theoretical}$ is the prediction of a theoretical model under the same conditions as the inputs of the neural network. The theoretical model can be derived based on physics-of-failures (Xu, 2021). It can also be established empirically based on previous experiments/observations (Gray, 2021). A custom loss function consists of the mean absolute error function and the physics-informed error. The physics-informed error introduces physical constraints in the neural network with the help of a theoretical model. The physics-informed error is calculated by taking the absolute difference of the predicted value and the theoretical estimate $y_{theoretical}$. Here, $y_{theoretical}$ can be derived from theory or be an empirical model derived from historical data. Since the objective of the loss function is to minimize the loss, the minimal value of the physics-informed error corresponds to the best theoretical fit. NN-I adopts this knowledge-constrained loss function to provide filtered estimates. These filtered estimates are known as neural filtered values. They are fed as an input to NN-II which performs the task

of predicting the RUL. In testing, NN-I is fed the live experimental data collected through sensors and the raw data is then filtered through the physics-embedded structure which can then be used to perform RUL estimation.

2.2. Neural Network – II

Neural Network II (NN-II) uses the obtained neural filtered estimates as an input to predict the RUL, which is the output of the two-stage network. The neural filtered estimates of the independent variables which are identified precursors for the degradation of the system, can be used to calculate the RUL. Neural Network II consists of a 3-layer neural network which employs Long-Short Term Memory, which uses a sliding window technique to predict RUL for a given time window. The NN-II network was constructed with one LSTM layer (16), two dense layers (8 and 1 neurons, respectively), and multiple dropout layers. The hidden layer and the output layer adopted a piecewise linear function (ReLU). NN-II assumes no underlying physical knowledge for RUL explicitly. As such, the mean absolute error loss was used as the loss function for this network. The theoretical RUL was calculated as follows:

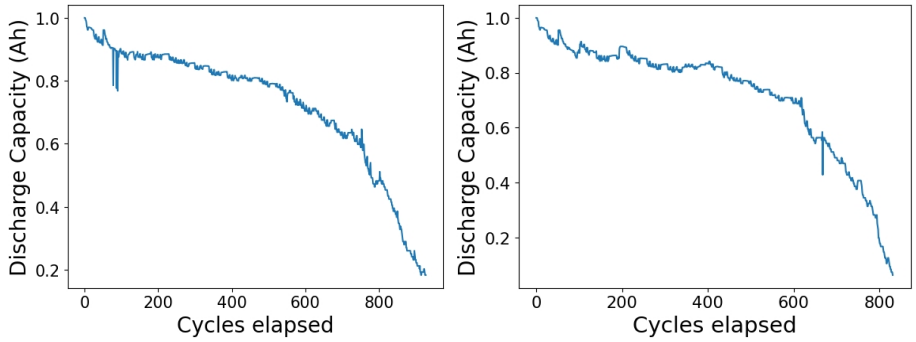
$$RUL = End\ of\ Life\ (EOL) - Number\ of\ cycles\ elapsed.$$

After the neural estimates are labeled with the theoretical RUL, NN-II performs a supervised learning task where the objective is to predict the RUL for the test data given a window of data points. The neural filtered estimates of the raw data collected is passed to NN-II where it continuously provides an estimation of the RUL for a given window of data points.

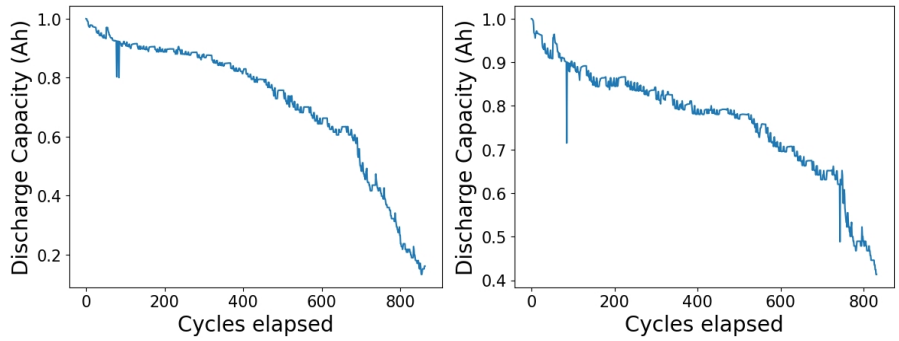
3. Case Study - RUL prognostics for lithium prismatic batteries

To illustrate our proposed 2-phase Neural Network architecture for RUL prediction, we consider the battery dataset available at the public repository CALCE (University of Maryland) (Wei He, 2011). This dataset contains a total of four batteries (CS2_35, CS2_36, CS2_37, CS2_38) which are cycled at a constant current protocol of 1C. For each battery, the following measurements are recorded: the charging capacity, constant current constant time (CCCT), constant voltage constant time (CVCT), discharging capacity, resistance. These measurements are available until the failure of the batteries. Here, a battery failure is defined as the first moment the capacity of this battery is below 80%.

The State of Health (SOH) of a battery at a given cycle is determined based on the maximum capacity achieved by discharging this battery from (100%) to (0%) charge in the considered cycle. We note that in the dataset, batteries undergo complete charge and discharge cycles. Moreover, the nominal capacity is 1.35 Ah for all four batteries in the dataset.



(a) (b)



(c) (d)

Fig. 2. (a) Discharge capacity over time for CS2_35; (b) CS2_36; (c) CS2_37; (d) CS2_38.

In line with existing research (Ma, 2019), we consider the discharge capacity as the health indicator for the batteries. The discharge capacity is monitored throughout the battery's discharge cycles. Fig 2. shows a plot of the discharge capacity variation over time for the four batteries considered in the dataset.

3.1. Integrating physical knowledge

Polynomial and exponential models are widely used for modeling battery capacity degradation (Micea, 2011; Xing 2013). In this study, we take the widely accepted double exponential model as the physical model for the degradation path, as shown in Eq. (2). For the sake of comparison, both traditional and physics-informed frameworks were employed. The traditional framework makes use of a standard mean absolute error function to train the model. In contrast, the physics-informed framework makes use of a knowledge-constrained loss function. In this manner, the experimental data is filtered and simultaneously knowledge is embedded into the model:

$$y(x) = ae^{bx} + ce^{dx}, \tag{2}$$

where $y(x)$ is the capacity of the battery, x is the cycle number, and a > 0, b < 0, c < 0, d > 0 are model parameters which are to be estimated. The coefficients of the exponential model in eq. (2) are estimated by fitting the curve with the least square method to the curves used for training during cross-validation. We note that the test data is only used for prediction and thus no coefficients were inferred using it. After the coefficients of the model are calculated, the model calculates the empirical value of the discharge capacity at every cycle during the training process of the model. The physics-informed error uses the empirical value at every cycle and calculates the custom loss.

4. Numerical Results - RUL prognostics for lithium-prismatic batteries

We apply our 2-phase Neural Network approach for RUL prediction for the four batteries in the CALCE dataset. A 4-fold cross validation is performed for the training and testing of the 2-phase neural network. As such, the training data used for a certain fold is only passed through the network to predict the RUL. It does not update weights and biases nor is it used to infer the coefficients for the theoretical model.

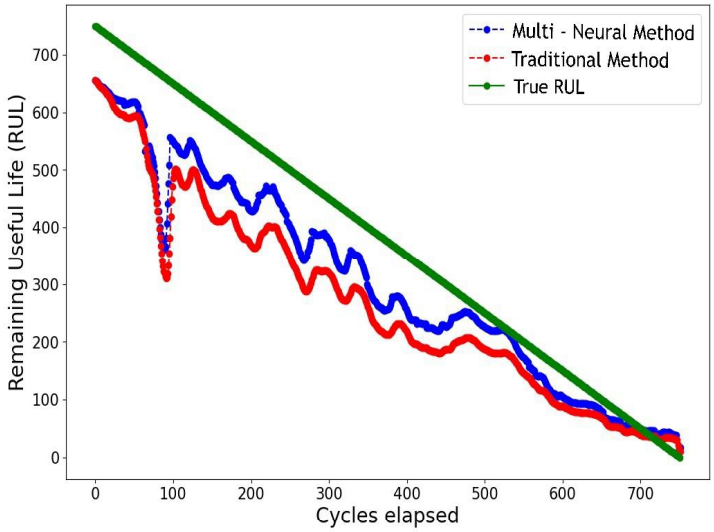


Fig. 3. RUL Predictions vs. the True RUL.

Fig. 3 shows the predicted RUL using the physics-informed prognosis framework versus the traditional approach where CS2_38 is used for testing. The average loss for the traditional approach is 101.09 cycles whereas the average loss for the two-phase method is 71.83 cycles. The loss for the neural filtered approach using embedded physical knowledge is lower compared to the traditional method and the error decreases continuously as it gets closer to failure. Table 1 shows the average values of loss for RUL prediction performed for multiple experiments with a 4-fold cross validation. The table compares the RUL loss with and without physical knowledge.

Table 1. Loss of the RUL prediction (cycles).

	Traditional model	Physics-informed model
Fold-1	132.931	129.048
Fold-2	118.736	90.318
Fold-3	69.361	67.457
Fold-4	189.087	185.295
Average value	127.528	118.029
Standard deviation	49.259	51.547

Figures 4 and 5 illustrate the fitting for the discharge capacity of the battery with and without physical knowledge after the values were obtained from NN-I. The loss with physical knowledge was 0.0483 and without was 0.0477. Multiple experiments with a 4-fold cross validation were performed. The average values are shown below in Table 2.

Table 2. Loss for discharge capacity.

	Traditional model	Physics-informed model
Fold-1	0.022834	0.022283
Fold-2	0.047136	0.048865
Fold-3	0.041240	0.036540
Fold-4	0.053375	0.052791
Average value	0.041146	0.040119
Standard deviation	0.013175	0.013759

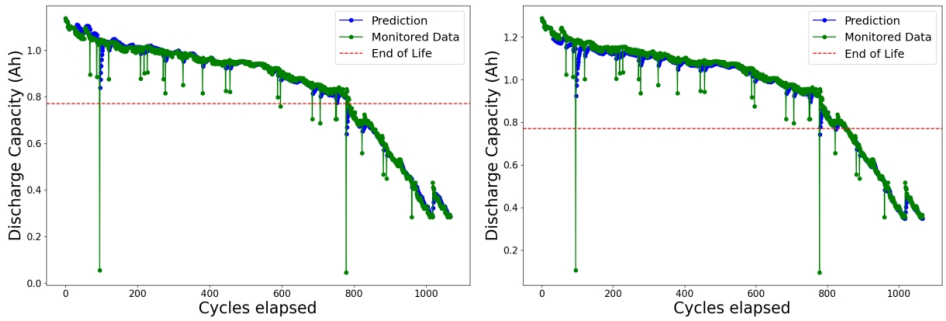


Fig 4. (a) Capacity Prediction with Physical Knowledge; (b) Capacity Prediction without Physical Knowledge.

It is interesting to note that the loss is higher while filtering the discharge capacity data using physical knowledge than without. However, the exact opposite phenomenon takes place while predicting the RUL. The inference from this result is that when physical knowledge is introduced, performance of NN-I slightly deteriorates as the physical constraints prevent overfitting of values and provide better theory-affirming estimates. This is favorable, as the performance while predicting RUL slightly increases.

Conclusion

This paper proposed a physics-informed two-phase neural network to predict the RUL of complex systems. This proposed multi-neural network provides a provision for filtering and embedding physical-knowledge simultaneously. The knowledge is inferred from a theoretical or an empirical model which describes the dynamics of the system. The knowledge is embedded in the first network which provides filtered estimates of the data to the second network which performs the task of predicting RUL. The proposed network was applied to predicting the RUL of prismatic batteries. An empirical model was derived that captured the degradation of the battery over time. The empirical model worked jointly with NN-I to provide physics-informed estimates of the data by using a custom loss function that uses physics-informed error. NN-II made use of these filtered estimates to predict the remaining useful life of the battery.

With the introduction of physical knowledge into the architecture, performance of NN-I slightly decreased. This implied that during the training process, the physical constraints prevented overfitting of data. Furthermore, RUL prediction in NN-II improves when incorporating physical knowledge compared to its performance without knowledge. It should also be noted that it is possible to integrate knowledge into Phase II of the proposed method if it is derivable. If sufficient physical knowledge is available to establish a theoretical dependency between variables involved in NN-II, the loss function can be customized. For instance, in crack growth prediction, paris law can be used to theoretically establish the rate of crack growth over time. This can be used to predict the RUL of a system affected by fatigue crack failure (Fang and Sun, 2022).

Acknowledgements

The participation of Aditya Sanju and Zhiguo Zeng to this project is financially supported by ANR under contract number ANR-22-CE10-0004. Zhiguo Zeng and Anne Barros are also partially supported by the Chaire of Risk and Resilience of Complex Systems (Chair EDF, SNCF and Orange).

References

Bhat, Darshankumar, Stefan Muench, and Mike Roellig. 2023. Application of Machine Learning Algorithms in Prognostics and Health Monitoring of Electronic Systems: A Review. e-Prime-Advances in Electrical Engineering, Electronics and Energy: 100166.

Zio, Enrico. 2022. Prognostics and Health Management (PHM): Where are we and where do we (need to) go in theory and practice. Reliability Engineering & System Safety 218:108119.

Jardine, Andrew KS, Daming Lin, and Dragan Banjevic. 2006. A review on machinery diagnostics and prognostics implementing condition-based maintenance. Mechanical systems and signal processing 20.7: 1483-1510.

Xu, Yanwen, et al. 2022. Physics-informed machine learning for reliability and systems safety applications: State of the art and challenges. Reliability Engineering & System Safety: 108900.

Chao, Manuel Arias, et al. 2022. Fusing physics-based and deep learning models for prognostics. Reliability Engineering & System Safety 217: 107961.

Raissi, Maziar, Paris Perdikaris, and George E. Karniadakis. 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics 378: 686-707.

Y. He, H. Su, E. Zio, L. Fan and J. Zhang. 2022. A Physics-Informed Training Approach for Data-Driven Method in Remaining Useful Life Estimation, 2022 6th International Conference on System Reliability and Safety (ICSRS), Venice, Italy, 2022, pp. 500-504

Wang, Y.; Han, X.; Guo, D.; Lu, L.; Chen, Y.; Ouyang, M. Physics-Informed Recurrent Neural Networks with Fractional-Order Constraints for the State Estimation of Lithium-Ion Batteries. *Batteries* **2022**, *8*, 148.
Xu, Zhaoyi, and Joseph Homer Saleh. 2021. Machine learning for reliability engineering and safety applications: Review of current status and future opportunities. Reliability Engineering & System Safety 211: 107530.
Gray, C.S. and Watson, S.J., 2010. Physics of failure approach to wind turbine condition based maintenance. Wind Energy, 13(5), pp.395-405.
He Wei, Williard Nicholas, Osterman Michael, Pecht Michael. 2011. Prognostics of lithium-ion batteries based on dempster–shafer theory and the bayesian monte carlo method. J Power Sources 2011;196(23):10314–21.
Ma, Z.; Yang, R.; Wang, Z. 2019. A novel data-model fusion state-of-health estimation approach for lithium-ion batteries. Appl. Energy 2019, 237, 836–847.
Micea, Mihai Victor, et al. 2011. Online state-of-health assessment for battery management systems. IEEE Transactions on Instrumentation and Measurement 60.6: 1997-2006.
Xing, Yinjiao, et al. 2013. An ensemble model for predicting the remaining useful performance of lithium-ion batteries. Microelectronics reliability 53.6: 811-820.
X. Fang, G. Liu, H. Wang, Y. Xie, X. Tian, D. Leng, W. Mu, P. Ma, G. Li, 2022. Journal of Building EngineeringAIAA Journal, Ocean Eng. 266, 112996
Sun L, Huang X. 2022. Prediction of fatigue crack propagation lives based on machine learning and data-driven approach. J Ocean Engng Sci 2022.