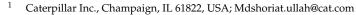




Article **Prediction of Lithium-Ion Battery Capacity by Functional Principal Component Analysis of Monitoring Data**

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Abstract: The lithium-ion (Li-ion) battery is a promising energy storage technology for electronics, automobiles, and smart grids. Extensive research was conducted in the past to improve the prediction of the remaining capacity of the Li-ion battery. A robust prediction model would improve the battery performance and reliability for forthcoming usage. In the development of a data-driven capacity prediction model of Li-ion batteries, most past studies employed capacity degradation data; however, very few tried using other performance monitoring variables, such as temperature, voltage, and current data, to estimate and predict the battery capacity. In this study, we aimed to develop a data-driven model for predicting the capacity of Li-ion batteries adopting functional principal component analysis (fPCA) applied to functional monitoring data of temperature, voltage, and current observations. The proposed method is demonstrated using the battery monitoring data available in the NASA Ames Prognostics Center of Excellence repository. The main contribution of the study the development of an empirical data-driven model to diagnose the state-of-health (SOH) of Li-ion batteries based on the health monitoring data utilizing fPCA and LASSO regression. The study obtained encouraging battery capacity prediction performance by explaining overall variation through eigenfunctions of available monitored discharge parameters of Li-ion batteries. The result of capacity prediction obtained a root mean square error (RMSE) of 0.009. The proposed data-driven approach performs well for predicting the capacity by employing functional performance measures over the life span of a Li-ion battery.

Keywords: lithium-ion (Li-ion) battery; functional principal component analysis (fPCA); battery monitoring data; state-of-health (SOH) diagnosis; LASSO regression

1. Introduction

The lithium-ion (Li-ion) battery is an integral part of many of our available systems, such as those used in laptops, cell phones, and the aerospace and power industries, and it has become crucial for the overall performance of such systems. As the demand for batteries is rising over the years, researchers are paying more attention to the health monitoring and prognostics of Li-ion batteries to avoid unexpected failures. Scientists are exploring state-of-the-art technologies to control the operating conditions and predict replacement intervals for batteries, aiming to improve the system reliability and consistency.

Over the years, several studies have been conducted to develop prediction algorithms for the state-of-health (SOH) of Li-ion batteries by the prognostics research community. Model-based and data-driven approaches are the main fields of study. The data-driven model is a method for mapping the relationship between the available observations and hidden variables using a framework built on obtainable performance measures [1]. Conventional approaches to battery prognostics mostly focus on exploring the SOH and stateof-charge (SOC) by employing battery capacity data [2,3]. These traditional approaches using capacity degradation data and theoretical assumptions frequently contribute to



Citation: Shoriat Ullah, M.; Seo, K. Prediction of Lithium-Ion Battery Capacity by Functional Principal Component Analysis of Monitoring Data. *Appl. Sci.* 2022, *12*, 4296. https://doi.org/10.3390/ app12094296

Academic Editors: Oriele Palumbo, Giovanni Dimauro, Rosalia Maglietta and Vito Renò

Received: 20 March 2022 Accepted: 21 April 2022 Published: 24 April 2022

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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). measurement inaccuracies, which may result in a battery failure [4]. However, these inaccuracies have compelled researchers to develop advanced prediction methods such as simulation, physical cell degradation, and data-driven prediction approaches [5]. Following the substantial prospects of Li-ion batteries, extensive research has been conducted to predict the remaining life cycles of Li-ion batteries using capacity degradation to improve battery performance and reliability. A comparative study was conducted for predicting Li-ion battery residual lifetime based on the Bayesian approach [6]. The study developed a non-parametric model which considered the mean of residual lifetimes. The study concluded that the Bayesian approach more accurately provides prediction results based on the confidence interval. However, researchers have seldom tried using other performance measures, such as temperature, voltage, and current observational data, to predict the capacity, although such measurements are as equally significant as capacity degradation for data-driven model development [7].

The study presented in this article focused on these issues by developing an empirical model based on Li-ion battery capacity degradation that is affected by the ambient environment and load condition. An effective prognostic algorithm should be able to predict the remaining useful life or capacity using the past life cycle data of battery performance. In this study, we aimed to predict the capacity of Li-ion batteries using a data-driven prognostics algorithm supporting uncertainty representation and management. During the study, the monitored data of the Li-ion battery were extracted as a form of a function due to the Li-ion battery's cyclic orders. While developing the model, the study addressed the effect of current, voltage, and temperature on the capacity degradation by applying the functional principal component analysis (fPCA) to predict the remaining capacity of a battery. Unlike the study of Wang and Mamo [8], where such monitoring data, i.e., current, voltage, and temperature, were included in the prediction model as a form of averaged quantities for each cycle, we identified the dominant models of functional variation using the framework of dimension reduction techniques. The battery monitoring observations collected from NASA Ames Prognostics Center of Excellence repository are used to illustrate our method. A notable contribution of the study is the proposal of a data-driven model that includes battery condition indicators, such as voltage, current, and temperature, and employs the dimension reduction statistical technique fPCA.

2. Literature Review

The fPCA technique has been used frequently for analyzing functional data such as magnetic resonance imaging (MRI) data, weather data, and stock exchange trends [9–11]. Significant research has been undertaken using fPCA, and the method helps to analyze continuous functions and enables the extraction of key features that epitomize dominant aspects of the original dataset [12]. In the field of bioinformatics, fPCA plays a crucial role in the analysis of time-course expression data by reducing the dimensionality of measurements without losing the generality [13]. Moreover, the data analysis enables the prediction of individual smooth trajectories, whereas limited measurements are available with the aid of asymptotic consistency and distribution [14]. Ramsay and Silverman [15] demonstrate several functional data analyses with the help of fPCA, in which different types of functional data are discussed. Roughness penalties are used to estimate the mean and covariance of functions in the analysis of the annual cycle of monthly climate data [16]. Detailed and comprehensive descriptions of functional data analysis, including prediction modeling, were discussed in a published book [15].

The method of analyzing functional data using fPCA has subsequently evolved significantly due to the varieties and complexities of functional data. In the prediction of multidimensional unbalanced functional data of protein structures, fPCA is used with regularized Gaussian basis functions [17]. The statistical tool was also applied to study the seat-to-stand movement of two separate groups, namely, osteoarthritis patients and healthy subjects. Human movement was studied by retaining all of the information for further analysis and the analysis was an extension of multivariate principal component analysis [18]. A detailed data-driven fPCA model utilizing a local quadratic smoothing function for Li-ion prognostics was used to measure mean functions [19]. The study presented a detailed model of longitudinal battery data through eigenfunctions and estimated variance and covariance functions with a combination of B-splines. This extensive research verified that a more comprehensive conclusion could be provided by fPCA than traditional discrete data analysis methods when datasets are continuous functions [12].

A distinct research scope can be determined for a data-driven prognostic model of Li-ion batteries based on literature reviews and past studies. Table 1 demonstrates the classification of the research scope.

Table 1. Literature of data-driven models' classification. The check mark indicates corresponding models used in each reference item.

| Authors | Data-Driven Models | | | | | | | | | | |
|-----------------------------------|------------------------|---------------------|------------------|--------------------|-------------------------------------|-------------------------|-------------------|------------------------------|--------------------------------|-------------------|---------------------|
| | Bayesian Regression | Gaussian Process | Kalman Filter | Particle Filter | Particle Swarm Op- timization | Autoregressive Based | Neural Network | Support Vector Machine | Relevance Vector Machine | Functional PCA | LASSO Regression |
| Hu et al., 2016 [20] | 1 | | | | | | | | | | |
| Patil et al., 2015 [21] | | 1 | | | | | | 1 | | | |
| Zheng et al., 2018 [22] | | | 1 | | | | | 1 | | | |
| Mavroforakis et al., 2006 [23] | 1 | | | | | | | 1 | | | |
| Long et al., 2013 [24] | | | | | 1 | 1 | | | | | |
| Kirk, 2014 [25] | 1 | | | | | | 1 | | | | |
| Nuhic et al., 2013 [26] | | | | 1 | | | | 1 | | | |
| Qin et al., 2015 [27] | | | | | 1 | | | 1 | | | |
| Zhao et al., 2018 [28] | | | | | | | | 1 | 1 | | |
| Richardson et al., 2017 [29] | 1 | 1 | | | | | | | | | |
| Xian et al., 2014 [30] | | | | 1 | | | | | 1 | | |
| Cheng et al., 2015 [6] | 1 | | | | | | | | | 1 | |
| Lin et al., 2017 [31] | | | | | | | | | | 1 | |

As can be seen from Table 1, much of the work regarding Li-ion batteries has used support vector machine (SVM), Bayesian regression, and machine learning (ML) algorithms to develop an empirical model. The current study took a novel approach, adopting fPCA to extract the feature from the dataset existing in the form of a function, and used LASSO regression, a penalized regression model, to fit better models by shrinking the model coefficients. The combination of fPCA and LASSO regression for analyzing functional monitoring data has not been used in previous studies and remains unexplored to date.

3. Methodology

The data used in this study were obtained from a publicly available data repository of the NASA Ames Prognostic Center of Excellence (PCoE) [32]. The study was conducted utilizing the extracted data from the NASA experimental battery No. 7, which was run through three different operational profiles, namely, charge, discharge, and impedance at room temperature. However, the capacity degradation study of Li-ion batteries requires voltage, current, and temperature to be measured during the discharge phase. Discharge was carried out at a constant current level of 2 A until the voltage dropped to 2.2 V. Repeated discharge cycles result in accelerated aging, and the process was halted once the battery reached its end of life (i.e., 30% rated capacity).

Suppose that a battery has been used for *N* charge–discharge cycles. The study defined the training data as $D_{train} = (X_{train}, Y_{train})$ where $X_{train} = \{v_{ij}, c_{ij}, t_{ij}, i = 1, ..., N, j = 1, ..., m_i\}$, which includes the monitoring measurements of voltage, current, and temperature for the first *N* cycles at m_i time points, and $Y_{train} = \{y_i, i = 1, ..., N\}$, the battery capacity data for the corresponding cycles, as the target. Based on the training data, we aim to

predict $D_{test} = (Y_{test}) = \{y_i, i = N + 1, ..., N + P\}$ the battery capacity for forthcoming *P* cycles. Note that the testing data does not include X_{test} as the monitoring observations are not available when the prediction is made in real applications. We instead attempt to predict $X_{test} = \{v_{ij}, c_{ij}, t_{ij}, i = N + 1, ..., N + P, j = 1, ..., m_i\}$ based on X_{train} , and use the predicted monitoring measurements as the input of the prediction model.

Figure 1 shows the graphical representation of the prediction model building and testing. For the model training, the functional principal component (fPC) scores are extracted from the first *N* cycles of voltage, current, and temperature measurements. These fPC scores are utilized to predict the battery capacity via the least absolute shrinkage and selection operator (LASSO), which is a penalized regression procedure used to fit the model by shrinking the coefficient to zero; this results in a biased prediction outcome with low prediction variance and enhanced prediction accuracy. For the model testing, we use the simple linear regression for each time index to predict forthcoming *P* cycles of monitoring variables based on preceding discharge cycles. Subsequently, fPCA is employed to extract the fPC scores from each predicted cycle of voltage, current, and temperature. The trained regression model is applied to predict the Li-ion battery's remaining capacity for cycles N + 1 to N + P. The result from the proposed model provides comparable accuracy throughout different cycling conditions over the life span of a Li-ion battery.

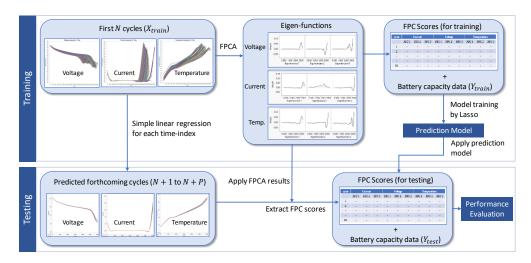


Figure 1. Graphical representation of workflow.

3.1. Functional Principal Component Analysis (fPCA)

The fPCA technique is an approach used to reduce the dimensionality of large datasets while helping to enhance interpretability, yet loses minimum information from the data. Herein, we briefly introduce the main idea of fPCA with an example of voltage measurement data v_{ij} . The fPCA can be thought of as an extended version of the traditional multivariate principal component analysis (PCA) with infinite-dimensional vectors, i.e., the function. To apply the fPCA, the data has to be given in the form of a smooth function. As the voltage data are discrete measurements over time, we first attempt to represent v_{ij} as a function $v_i(t)$ using a B-spline basis expansion with an appropriate number of knots.

The fPCA aims to find weight functions $\phi(t)$ that mostly explain the function-tofunction variabilities. The first functional principal component $\phi_1(t)$ is chosen to maximize the mean square $\sum_{i=1}^{N} \xi_{i1}^2 / N$ where:

$$\xi_{i1} = \int \phi_1(t) v_i(t) dt \tag{1}$$

with the constraint of the unit squared norm $\int \phi_1(t)^2 dt = \|\phi_1\|^2 = 1$. The second and subsequent fPCs can also be found by solving the same optimization problem with the additional orthogonality constraints of $\int \phi_k(t)\phi_m(t)dt = 0$, k < m. Let us define the

covariance function $G(s, t) = \sum_{i=1}^{N} v_i(s)v_i(t)/(N-1)$; then, it can be shown that the above optimization problem is reduced to the following eigen-equation:

$$\int G(s,t)\phi(t)dt = \lambda\phi(s)$$
(2)

where $\phi(\cdot)$ is an eigenfunction and λ is an eigenvalue. This continuous functional eigenanalysis problem can be solved by an approximately equivalent matrix eigen-analysis task. For more details, see chapter 8.4 of Ramsay and Silverman [15]. It can also be shown that each curve of $v_i(t)$, i = 1, ..., N is approximated by the expansion in terms of a small number of orthonormal basis functions ϕ 's by the following form:

$$v_i(t) \cong \mu(t) + \sum_{k=1}^K \xi_{ik} \phi_k(t)$$
(3)

where $\mu(t) = \sum_{i=1}^{N} v_i(t)/N$ is the mean function, $\xi_{ik} = \int \phi_k(t)v_i(t)dt$ is the *k*-th fPC score, and $\phi_k(\cdot)$ is the *k*-th eigenfunction. The same procedure can be conducted for the current and temperature curves. In our research, we extracted five fPC scores from each curve of voltage, current, and temperature. These 15 fPC scores for each cycle are used as the input features of the battery capacity prediction model.

3.2. Prediction Model Building and Testing

The aim of the study was to build a model that can be used to predict Li-ion battery capacity using fPCA. The following is the process of capacity prediction model building and testing.

- (a). The monitoring data of the Li-ion battery comprise 168 cycles of voltage, current, and temperature. To begin, we considered the initial N = 100 cycles as training data to build a prediction model.
- (b). The original discretized measurements are transformed to smooth curves by applying the B-spline basis expansion. The number of knots is chosen, for each of voltage, current, and temperature, such that the fitted model has the lowest BIC value.
- (c). The fPCA technique is performed on each monitoring variable, and the mean function $\mu(t)$, fPC scores ξ_{ik} , k = 1, ..., K, and corresponding eigenfunctions are obtained for each predictor. These fPC scores characterize the status of the battery at the corresponding cycle.
- (d). The LASSO regression model is trained based on fPC scores. The LASSO complexity parameter is chosen by the K-fold cross-validation with 5 folds.
- (e). To test the model, the monitoring variables' measurements for the forthcoming P = 20 cycles are predicted. Simple linear regression was used for this task for each time point. For the voltage measurements for a time point of j = 1, for example, we fit the following model to the initial 100 cycles of data:

$$v_{i1} = \beta_0 + \beta_1 i + \varepsilon_{i1}, \ i = 1, \dots, 100$$
 (4)

Then, the fitted model is extrapolated to produce \hat{v}_{i1} , i = 101, ..., 120. This process is repeated for each time point of $j = 1, ..., m_i$. Merging these resulting responses, we obtain the predicted 20 cycles, which are almost indistinguishable from actual cycles. The B-spline with the number of knots learned by the training data is applied to these predicted measurements.

- (f). Using the eigenfunctions obtained from the training phase, the fPC scores are extracted from each predicted curve.
- (g). The prediction of \hat{y}_i , i = 101, ..., 120 are obtained by LASSO model obtained in (d) and compared with the true battery capacity values to evaluate the model performance.

The functional data explorer from the software JMP Pro 14 [33] was used to implement the tasks mentioned above, except (e), which provides useful features to deal with functional data provided as discrete measurements. Task (e) was conducted using R [34].

4. Experimental Results

The fPCA model was employed to analyze the initial 100 cycles of data of voltage, current, and temperature to provide fPC scores and eigenfunctions. Based on the BIC value, the cubic spline was adopted to fit the model. We set the number of knots to 35, which provided better results than other options. Figure 2 illustrates examples of the fitted B-spline basis expansion model for the first 25 cycles of voltage curves.

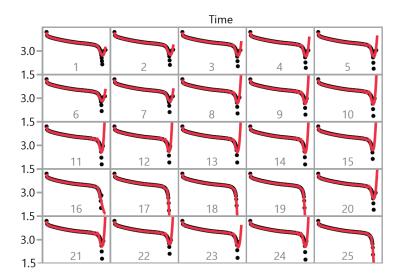


Figure 2. B-spline fitted for the first 25 cycles of voltage curves.

The fPCA for voltage provided fPC scores and eigenfunctions, where the first fPC was responsible for 75.4% of the data variation and the second fPC was accountable for 21.1% of the data difference. Similar results were found in the case of current. The first fPC was responsible for about 67.2% of the variation and the second fPC was responsible for 29.2% of the variation in the functional current data. The temperature shows multiple fPCs for the variation, where the majority was covered by both the first and second fPCs. The first fPC was responsible for 42% and the second fPC covered 33% of data variation. Figure 3 demonstrates the corresponding eigenfunctions against fPC scores that we obtained from voltage, current, and temperature.

The battery capacity prediction begins with predicting the voltage, current, and temperature of the forthcoming cycles using simple linear regression. We obtained similar shapes of cycles as those of the preceding 100 cycles. Figure 4 illustrates the predicted 20 cycles of current, temperature, and voltage.

The fPC scores that we obtained through the model are the input for the generalized regression model, where we used adaptive LASSO regression with five-fold cross-validation. LASSO was used to train the preceding fPC scores with their corresponding capacity and to help predict the capacity based on the fPC scores of predicted cycles. We considered the initial 100 cycles as a training dataset, and the predicted 20 cycles were used for model testing. Figure 5 shows the plot for predicted capacity versus capacity residuals for the training dataset.

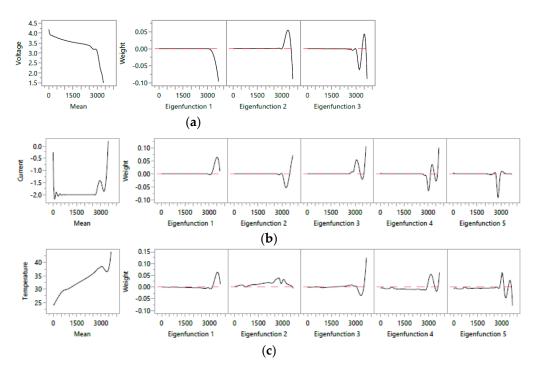


Figure 3. Graphical demonstration of the fPCA for monitoring data. The mean functions and eigenfunctions of (**a**) voltage, (**b**) current, and (**c**) temperature are displayed.

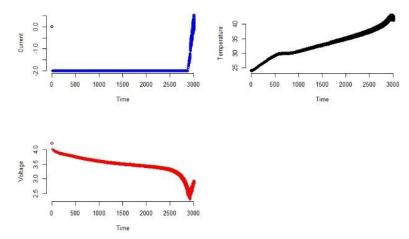


Figure 4. The predicted 20 forthcoming cycles of current, temperature, and voltage.

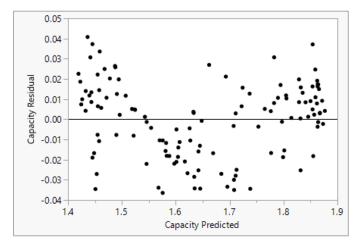


Figure 5. Actual versus predicted capacity for training and testing datasets.

As shown in Figure 5, the residuals are randomly distributed, which corroborates the model validity and facilitates credible prediction outcomes. The result provides evidence that the capacity prediction appears to be closer to the actual curve and is more accurate with more capacity data if available for further updates.

Initially, the study considered 100 cycles and predicted the capacity for the subsequent 20 cycles. We continued the process considering 120 cycles and predicted the following 20 cycles. This process helped us to check the model and verify its accuracy of prediction. Figure 6 shows the outcome of the model capacity from cycle 1 to 120. The fitted capacity curve is color coded, so that fitted capacity and predicted capacity are evident.

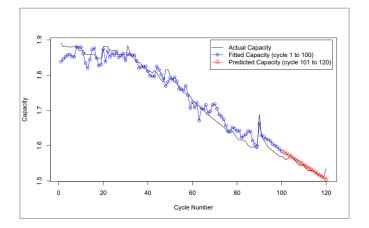


Figure 6. Capacity prediction results of Case 1.

The errors, such as root mean square error (RMSE) and mean absolute percentage error (MAPE), show that the model works well at the beginning, when both the RMSE and MAPE are minimal. However, both errors increase as the model predicts end cycles. Table 2 illustrates the prediction performances using different training cycles for three separate cases.

| Criteria | Case 1 | Case 2 | Case 3 | |
|----------|----------------|----------------|----------------|--|
| | Training cycle | Training cycle | Training cycle | |
| | 1–100 | 1–120 | 1–140 | |
| | Testing cycle | Testing cycle | Testing cycle | |
| | 101–120 | 121–140 | 141–160 | |
| RMSE | 0.009 | 0.02 | 0.04 | |
| MAPE (%) | 0.44 | 1.74 | 3.18 | |

Table 2. Prediction performance of battery No 7 for three separate cases.

Note that the small error values from MAPE and RMSE represent better accuracy, as shown in Table 2. The study considered three scenarios to develop the empirical model and test the dataset capable of predicting the capacity at any point of the battery's lifespan. For the first case, we took the first 100 cycles to obtain the mean function and derive eigenfunctions sufficient to explain the overall variation with the help of LASSO regression. The derived fPC scores were utilized to predict the forthcoming 20 cycles. Case 2 demonstrates the first 120 cycles for the training purpose, whereas Case 3 depicts the first 140 cycles for the initial training. Each time, the model tested and predicted the subsequent 20 cycles using the training fPC scores. The results indicate that fPCA prediction model based on current, voltage, and temperature performs better at the beginning stage rather than at the later-period prediction of the battery life. The higher MAPE (%) for the last case is due to the inconsistent data trend of the monitored data, which is a common behavior of Li-ion batteries under load at the end of the lifespan. The dataset only comprises 161 cycles of monitored data since it reaches to the end of its lifetime.

5. Conclusions

A capacity prediction method for the Li-ion battery based on fPCA using LASSO regression is demonstrated. The prediction model is applied using fPCA, and helps to predict the capacity of the Li-ion battery. LASSO regression is employed to explore the fPC scores that the study obtained from the fPCA model, and thus provide predicted cycle capacity. From the experiment results, the study observed that the proposed model based on fPCA can effectively predict Li-ion battery capacity. The statement verified by the performance of errors such as RMSE and MAPE proves that the model can deliver higher prediction accuracy.

Some limitations of the model were also observed during analysis since the model does not perform equally throughout the life cycle. Future works will be conducted considering more sophisticated curve predictions for voltage, current, and temperature rather than simple linear regression. Another area for further research is the consideration of the influence of the battery regeneration phenomenon on the capacity prediction in the fPCA model. In conclusion, we believe that the fPCA model based on voltage, current, and temperature is a potentially useful tool for capacity prediction of Li-ion batteries and can deliver better accuracy than other published conventional approaches.

Author Contributions: Conceptualization, K.S.; methodology, M.S.U. and K.S.; software, M.S.U.; validation, M.S.U. and K.S.; formal analysis, M.S.U.; investigation, M.S.U. and K.S.; resources, M.S.U. and K.S.; data curation, M.S.U.; writing—original draft preparation, M.S.U.; writing—review and editing, K.S.; visualization, M.S.U.; supervision, K.S.; project administration, K.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: Publicly available datasets were analyzed in this study. This data can be found here: https://ti.arc.nasa.gov/tech/dash/groups/pcoe/prognostic-data-repository.

Conflicts of Interest: The authors declare no conflict of interest.

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