

Lithium-ion battery optimal RUL prediction combining LSTM and GANs

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A R T I C L E I N F O .

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Abstract

Lithium-ion batteries have emerged as a prevalent power source in a variety of industries, including the electric vehicle (EV) sector due to their higher energy density and low self-discharge. With the use and passage of time, batteries degrade and eventually die, endangering the integrity of the objects they power. An accurate prediction of the remaining useful life (RUL) of lithium-ion batteries is therefore essential to maximize the efficiency of their use and ensure safety. For this purpose, a deep learning-based approach trained on the widely used Oxford battery degradation dataset with the help of generative adversarial networks (GANS) has been implemented. The designed network consists of a long-short-term memory (LSTM) architecture with the implementation of a stratification strategy and a custom loss function. The illustrative results show that the suggested approach can produce adaptable and reliable predictions of the RUL.

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1 Introduction

The advancement of Lithium-ion (Li-ion) batteries in recent years has transformed the field of energy storage. This type of energy source has emerged as the preferred choice for powering electronic devices. A major advantage of this type of energy storage is its high coulombic efficiency and fast charging capabilities [1, 2]. The lithium-ion battery has a range of applications and has had a significant impact on the automotive industry [3]. It has also expanded to other areas, such as aerospace [4] or photovoltaic [5] applications, offering even more optimal performance. However, the main limitation of lithium-ion batteries is their lack of ability to provide the high charging capabilities required for specific applica-

tions, such as transport and static energy storage [6].

Some of these drawbacks are because of the operating area of the batteries, which can lead to fast degradation or even safety issues, as commonly seen in the Electric Vehicle (EV) industry [7]. Restrictions in the voltage range can generate extreme amounts of heat due to overcharges, thus, the deposition of metallic lithium on the surface of the negative electrode is accelerated, leading to capacity failures. In short, these aspects can lead to: (i) reduced lifetime, (ii) fast degradation rate and (iii) safety problems.

To address these issues, there has been a growing interest in studying the reliability and management of Li-ion batteries, including the estimation of their remaining useful life (RUL) and the characterization of their performance degradation metrics like State of Health (SoH)

[8]. The most popular approaches include statistical model-based, artificial intelligence (AI)-based,

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physics-based, and hybrid approaches [9]. While each of these approaches offers several techniques for RUL prediction, this study specifically employs AI-based techniques, with Artificial Neural Networks (ANN) and Deep Neural Networks (DNN) being the main techniques used.

The main objective of this work focuses on RUL estimation of Li-ion batteries through ANN, customising the loss function and enhancing the predictive capabilities of these applications through synthetic data generation. Thus, a comparative study is made showing that the proposed approach is superior to the conventional RNN approaches.

2 Related Work

Physical-based approaches for RUL prediction are focused on the specific chemical and physical phenomena that affect battery conduct and find the details of performance evaluation. Although these have been widely used methods for the estimation of the RUL, the fitting of a perfect model for battery simulation presents great difficulty because of the multiple interactions between components that affect the degradation of the battery, particularly since degradation of the battery is active and nonlinear [9]. Since it is hard to observe a battery's inner conditions in real-time, an exact physical model is difficult to obtain [10].

Data-driven techniques, particularly Machine Learning (ML) and Deep Learning (DL) methods, have been found to be reliable for estimating RUL and SOH of Li-ion batteries. The ability of artificial neural network (ANN) approaches to learn nonlinear relationships between features has led to the development of many techniques for accurate RUL prediction [10], and even hybridization of diverse AI-based methods [11].

The field of deep learning has experienced substantial advancements, and various methodologies incorporating autoencoders have undergone various testing [12, 13]. However, there has been debate surrounding the trade-off between model interpretability and performance. Traditional, interpretable ML models such as kernel regression approaches have also been found to be effective for capturing non-linearity [14], but they require time-consuming feature engineering [15]. Deep learning approaches, particularly recurrent neural networks (RNN) such as Long Short-Term Memory (LSTM) networks, have been shown to produce the most favourable outcomes. In numerous studies, methods based on recurrent neural networks (RNNs) have demonstrated predictive accuracy with root mean square error (RMSE) values of less than 6 cycles in forecasting RUL [16–18].

RNNs have been widely used for sequence modelling tasks. However, their effectiveness is limited when the input sequence is long, as the sigma and tanh cells that make up RNNs are unable to learn relevant information from the input data. Long-term dependencies in the sequence can be effectively addressed by incorporating gate functions into the cell structure of LSTM networks [13]. Nevertheless, when dealing with large sequential data, the initial information of the sequence may be lost despite the use of gates [19]. To address this limitation, a new network architecture called the transformer has been proposed, which leverages the use of attention mechanisms to precisely remember the position of sequential data [20]. While initially developed for text, transformers have been shown to be effective for various types of sequential data. Several projects in this field have reported promising results [21, 22].

Despite the advantages of Deep Learning algorithms, certain challenges still exist that make their use difficult in certain scenarios. One such challenge is the loss of interpretability of results due to the generation of many relationships to make predictions [23]. Another challenge is the high number of parameters that these models generate, resulting in heavier models compared to traditional machine learning models. In addition to these, deep learning models suffer from the use of insufficient or unbalanced data. This problem is a particular obstacle for deep learning algorithms, which rely heavily on large datasets for promising results [24].

To address this issue, Generative Adversarial Networks (GANs) can be employed. GANs are a Deep Learning approach that involves generating synthetic data that closely resembles the provided data [25]. These techniques have been used in various domains, including Li-ion batteries, and have provided accurate results even with limited data availability. While GANs are commonly used for image datasets [26], their use in tabular data has also been studied [27]. GANs consist of two main components: a generator network and a discriminator network. The generator network learns to generate new samples that resemble the training data, while the discriminator network aims to distinguish between real and generated samples. During training, the two networks engage in a minimax game, where the generator tries to fool the discriminator, and the discriminator strives to correctly classify the samples. This game results in an iterative process that progressively improves the generator's ability to generate high-quality samples [28]. GANs employ various loss functions, with the most commonly used being the adversarial loss, which encourages the generator to produce samples that are indistinguishable from real data, and the

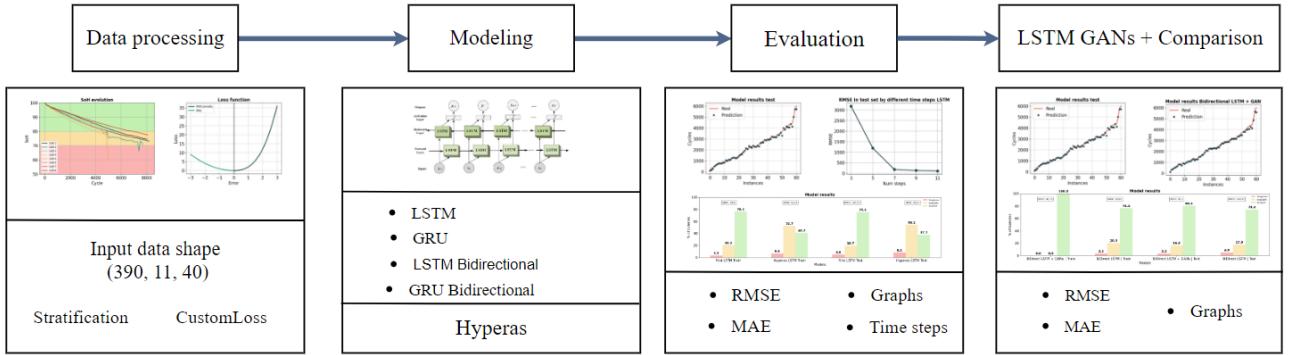


Figure 1. Summary of the whole process to achieve the results divided into 4 stages: Data Processing, Modeling, Evaluation and LSTM GANs + Comparison.

generator loss, which penalises the generator for generating low-quality samples [28].

Despite their success, GANs still have limitations, including instability during training, mode collapse (where the generator produces limited variations of samples), and challenges in evaluating and controlling the generated outputs. These limitations continue to be active areas of research to enhance the effectiveness and robustness of GANs [25].

3 Methodology

The methodology encompasses several key steps. Firstly, a data manipulation strategy is defined to ensure optimal utilisation of the dataset. Next, the selection process involves choosing the most suitable Remaining Useful Life (RUL) model from a range of algorithms, including LSTM, GRU, bidirectional LSTM, and bidirectional GRU. Subsequently, model evaluation is performed, wherein a custom loss function is employed in addition to commonly used metrics. Finally, leveraging the selected model, an approach is proposed to generate synthetic data using Generative Adversarial Networks (GANs), further enhancing the robustness and versatility of the developed model. As a summary of the methodology followed, Figure 1 depicts the developed strategies.

3.1 Dataset description

This work is based on the Oxford battery degradation dataset, which includes data from 8 small Li-ion pouch cells that were charged and discharged in a thermal chamber at 40 degrees Celsius. The dataset contains information on time, voltage, charge, and temperature, collected every 100 cycles [29].

3.2 Data processing

To develop a predictive model, the time, voltage, charge and temperature features obtained from the Oxford battery degradation dataset underwent a se-

ries of aggregations. These aggregations are mainly based on the most common statistical tendency measures. Each cycle's data was combined to form a representative dataset. Indicators were computed for voltage, charge, and temperature. Additionally, the state of health (SoH) of the batteries was estimated by comparing their maximum capacity in each cycle with their initial capacity. In short, the features extracted from the original data are the following:

- **Time.** Maximum and minimum values.
- **Voltage.** Maximum, minimum, mean, standard deviation, skewness and kurtosis coefficients.
- **Charge.** Maximum, minimum, mean, standard deviation, skewness and kurtosis coefficients.
- **Temperature.** Maximum, minimum, mean, standard deviation, skewness and kurtosis coefficients.
- **SoH.** Maximum value.

Both charge and discharge cycles were analysed, and relevant features were extracted from the original data. The target variable for the model development was the Remaining Useful Life (RUL) of the batteries. In total, the final dataset consisted of 390 rows and 41 columns, encompassing the RUL value. The RUL was measured by determining the number of remaining cycles before the SoH dropped below 80%.

Notably, different perspectives exist regarding the definition of a battery's End of Life (EOL). Some researchers consider it to be when the nominal capacity decreases by 20% [30], while others suggest that failures can occur when the decrease ranges between 20% and 30% of the nominal capacity.

Although the RUL calculation is based on a 20% decrease threshold, the study acknowledges that failures may occur in the 20-30% capacity decrease range. Therefore, Equation 1 defines the acceptance criteria for RUL prediction to be within the state of

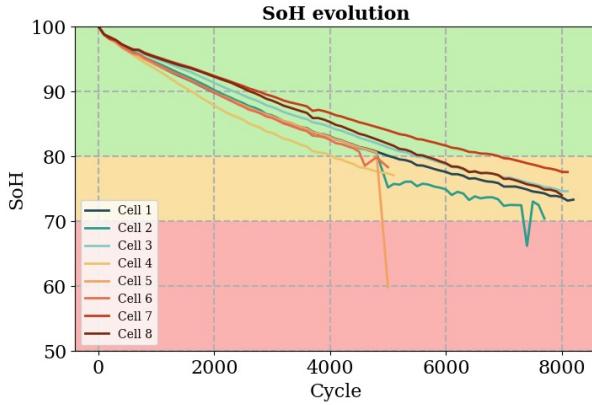


Figure 2. SoH evolution for every battery. The actual SoH of the battery is represented by three colors: red when $\text{SoH} < 70\%$, yellow when $70\% < \text{SoH} < 80\%$, and green when $\text{SoH} > 80\%$. The SoH decreases as the number of cycles increases.

health (SoH) range of 82% to 80%. This range ensures that predicted SoH values are not too close to the expected end of life (EOL) of the battery, but still within an acceptable range of use. To comply with these constraints, the parameters α , β , and γ were set to 70%, 80%, and 82%, respectively.

$$f(\text{SoH}) = \begin{cases} \text{Dangerous} & \text{if } \text{SoH} < \alpha \\ \text{Acceptable} & \text{if } \text{SoH} > \gamma \\ \text{Excellent} & \text{if } \gamma \leq \text{SoH} \geq \beta \end{cases} \quad (1)$$

Figure 2 shows a comparison of the SoH of the 8 cells, indicating that most of them fail when their degradation level exceeds 20%, lasting for about 8,000 cycles. However, some cells exhibit unconventional behaviour and fail after only 5,000 cycles. The 5th battery is particularly noteworthy as it experiences significant degradation during a few cycles, resulting in its EOL being at a degradation level close to 40%.

3.3 Training procedure

The current phase of the study has centred on employing Recurrent Neural Networks (RNNs) for predicting the Remaining Useful Life (RUL) of batteries. The training methodology for these algorithms has exhibited certain unique aspects. Initially, experiments were conducted using data from all 8 batteries. However, a strategy was devised to develop a model that could generalise its predictions for batteries beyond the training set. Additionally, the final model was retrained using data from only 7 cells to evaluate its predictive performance for the 6th battery.

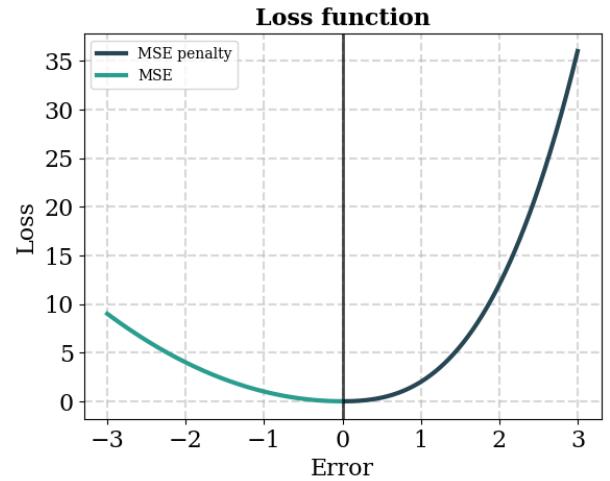


Figure 3. MSE custom loss function for penalising negative values. The penalty only affects the excess of cycles in the prediction.

3.3.1 Loss function

The development of a custom loss function has been an important aspect in training the algorithms. Algorithm 1 has been designed based on the Mean Squared Error (MSE); however, it penalises predictions that indicate a battery has more remaining cycles than it actually does. This can be seen in Figure 3, where the MSE increases as the prediction exceeds the actual RUL value.

Algorithm 1 MSE custom loss function

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1: function MSECUSTOMLOSS( $y_{true}$ ,  $y_{pred}$ )
2:    $difference = y_{pred} - y_{true}$ 
3:    $greater = max(difference, 0)$ 
4:    $greater = greater + 1$ 
5:   return  $MSE(difference) \times greater$ 
6: end function
```

An accurate prediction of battery cycles is crucial for safety in the context of electric vehicles (EVs), as over-predicting the remaining cycles of a battery can lead to dangerous situations. Under-predicting the remaining cycles may not be as dangerous but can still result in inconvenience for the vehicle's owner. Therefore, the appearance of predictions suggesting that a battery has more remaining cycles than it has could be quite dangerous in practice.

3.3.2 Stratification strategy

Regarding the training samples, a validation set has been extracted from the main set. The strategy for this includes two methods: (i) cell-based stratification, where the proportion of data batches belonging to each cell has been maintained in both training and test sets, and (ii) cycle-based stratification, where

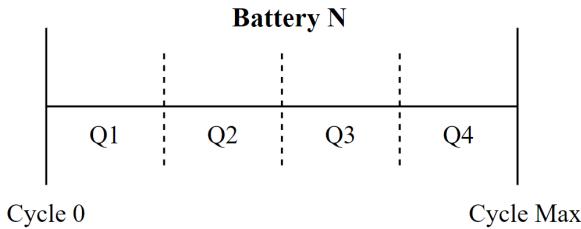


Figure 4. Quantile stratification for train and test sets.

the cycle of each data sample is considered and the distribution of cycle-labels is divided into quantiles to distribute the proportion of instances equally. An illustration of this method has been provided in Figure 4.

These two strategies have been aggregated in order to combine their effects. This combined method ensures that the algorithm will be provided with balanced data sets in both training and test stages, trying to avoid overfitting at certain cycles of batteries. The aim of this stratification lies in feeding the RNN with data that captures the most diverse patterns as possible, so that it could perform properly, regardless of the cell they belong to or their current cycle.

3.3.3 Data augmentation

As introduced in section 3.2, the dataset is far from the size standards used for training deep learning models. So, the inclusion of GANS has supported the training of the LSTM network explained in section 3.4. As stated in section 3.3.2, the training data has been divided into batches of equal size to feed the RNN. This set has been augmented to achieve completeness and diversity.

In the context of machine learning, completeness refers to the degree to which a dataset represents the entire population or phenomenon under study. On the other hand, diversity pertains to the variety and heterogeneity of the data within a dataset, which can significantly impact the accuracy and generalizability of a machine learning model. To generate and discriminate the batches, both the generator and discriminator components adopted an LSTM architecture. The performance of these components was assessed using the binary cross-entropy loss function, while the model's architecture also incorporated bidirectional LSTM layers, dropout strategies, and Leaky ReLU activation functions.

In total, 128 new batches, comprising (30%) of the training set, were generated through the GAN augmentation technique. This decision to allocate (30%) of the dataset to the generated batches was deemed

balanced, as it represents a substantial portion while still maintaining the real data as the majority group. By adopting this approach, the study seeks to strike a harmonious balance between incorporating synthetic data to enhance model training and preserving the authenticity and representativeness of the real data.

3.4 LSTM architecture

As stated in section 2, recurrent neural networks are among the cutting-edge approaches for time series prediction. To establish a baseline for further analysis, initial models were constructed using the main RNN methodologies, namely Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU), as their bidirectional variants [31]. Notably, the evaluation of these models' performance relied on the employment of two key metrics: Root Mean Squared Error (RMSE) and Mean Absolute Error (MAE). These metrics offer a comprehensive understanding of the model's behavior regarding the target variable.

Table 1, shows the lowest metrics obtained with the bidirectional Long Short-Term Memory (LSTM) model on both the training and validation sets. These models were exclusively trained using the original data. Subsequently, an optimization process was conducted to determine the optimal architecture and parameters for the proposed model. The chosen network configuration comprises a bidirectional LSTM layer with 624 neurons. The forward stage incorporates a LeakyReLU activation function with an alpha value of 0.3, while the backward layer utilises a PReLU activation function with 416 neurons. A recurrent dropout rate of 0.05 has been implemented. The Adam optimizer was selected, employing a low learning rate of 0.0001. The model was trained using stratified sets of the 8 batteries over 20,000 epochs, with a batch size of 16. The loss function implemented aligns with the one discussed in 3.3.1.

Furthermore, to determine the optimal number of time steps inputted into the network, several experiments were conducted for validation purposes. As depicted in Figure 5, the bidirectional LSTM achieved the lowest Root Mean Squared Error (RMSE) when trained with an 11-step-based approach. Additionally, this particular model underwent testing using the synthetic data generated in section 3.3.3.

4 Results and discussion

The algorithms employed in this study were also trained using the synthetic data produced by the LSTM-GANs. Ultimately, the GAN-based approach yielded slightly superior metrics, and the results obtained based on the prediction criteria outlined in Equation 1 were more robust. When utilizing

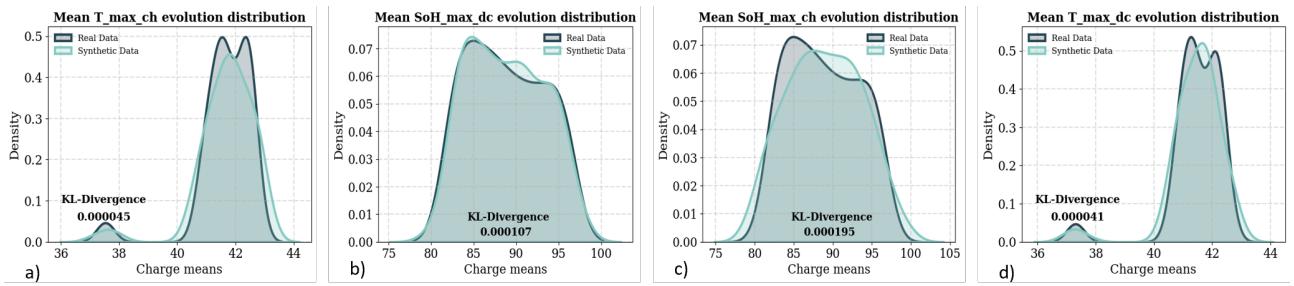


Figure 5. Synthetic data quality evaluation based on histograms and KL divergence.

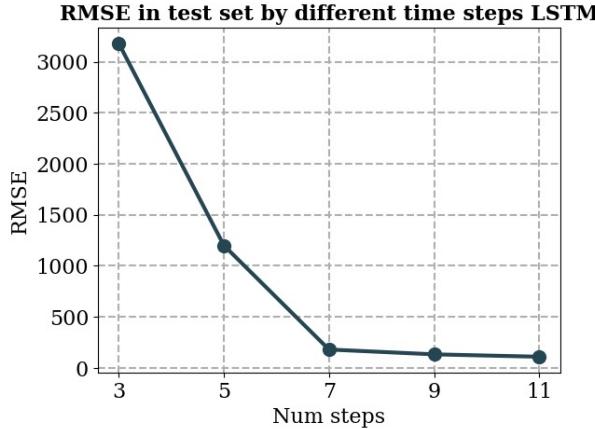


Figure 6. Performance of the algorithm when training with different time steps. RMSE is minimized with an 11-step-based training.

synthetic data, the proportion of accurate predictions was notably higher, as shown in Figure 7.

Figure 8 shows that the model typically avoids predicting negative values for any of the batteries. Moreover, the deviation between the predicted values and the actual values tends to be low for both positive and negative cases, with a mean cycle prediction deviation error of +73 and -23.5, respectively. The colour spans in the figure represent the actual State of Health (SoH) values for each cycle, indicating that a majority of the predictions fall within an acceptable prediction range in terms of battery health. Thus, it can be concluded that the trained algorithm effectively models the real context with accuracy, as evidenced by the R2 and RMSE metrics.

After proving the performance of the designed

Table 1. Results for every model with the most optimal architecture.

	Train RMSE	Train MAE	Val RMSE	Val MAE
<i>LSTM</i>	143.66	97.96	157.17	111.19
<i>GRU</i>	76.70	41.99	164.75	115.00
<i>BiD - LSTM</i>	49.54	36.26	108.57	76.9
<i>BiD - GRU</i>	45.28	21.93	111.72	74.86

Table 2. Training and Test metrics using LSTM and GANs architecture for the sixth battery prediction

	RMSE	MAE	R2	Custom Loss
<i>Train</i>	248.16	224.85	0.9538	19364305
<i>Test</i>	253.09	232.66	0.9407	20141576

model through Figures 7 and 8, the subsequent step consisted of training a model with the identical architecture but isolating the 6th battery. The entire data preparation procedure was replicated using all batteries except the 6th cell, including the incorporation of synthetic data generated by LSTM-GAN.

Although the obtained RMSE metric of 253 is higher compared to other observed studies [29], the algorithm's performance remains positive. Only 11 predictions in the test set exceeded the real Remaining Useful Life (RUL), accounting for (18%) of the predictions. Additional metrics, such as the R2 coefficient and the custom loss function presented in section 3.3.1, were evaluated in this stage. The results, presented in table 2, indicate that the proposed model effectively avoids overfitting.

Examining the final predictions for the 6th battery, as depicted in Figure 9, it can be observed that, excluding 2 of the final cycles, the remaining predictions fall within the space of excellent predictions. Notably, the predicted values do not exceed the real values, highlighting the efficacy of the self-made loss function. This indicates that the model achieves the desired generalization, as it avoids predictions beyond the theoretical End of Life (EoL). The model strikes a balance between metric-based performance and task-oriented performance.

5 Conclusions and future works

5.1 Conclusions work

This work introduces an LSTM architecture that, when combined with a custom loss function and data augmentation using LSTM GANs, demonstrates a superior approach compared to conventional RNNs. The integration of these techniques has resulted in

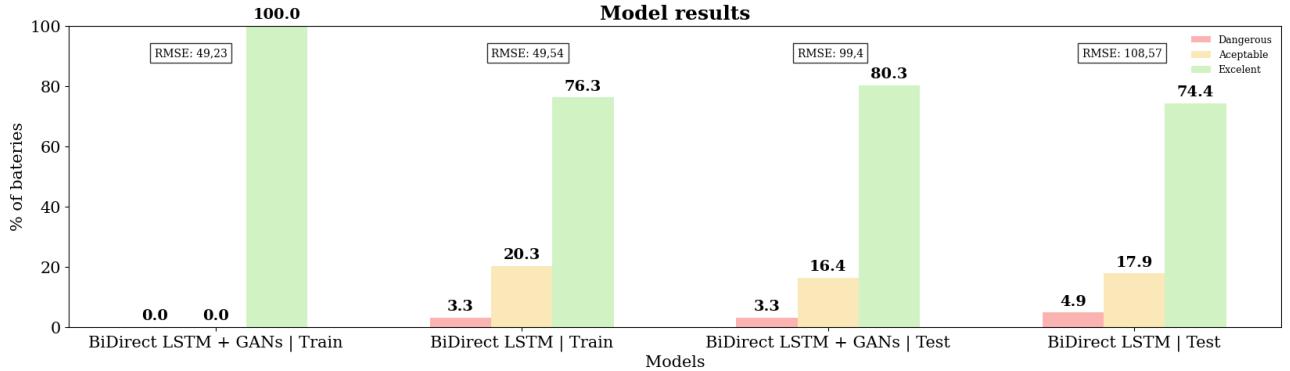


Figure 7. Representation of the performance of the model trained with original data and GAN- generated synthetic data. The figure shows the percentage of predictions rated as dangerous, acceptable and excellent as well as the total RMSE within train and test data.

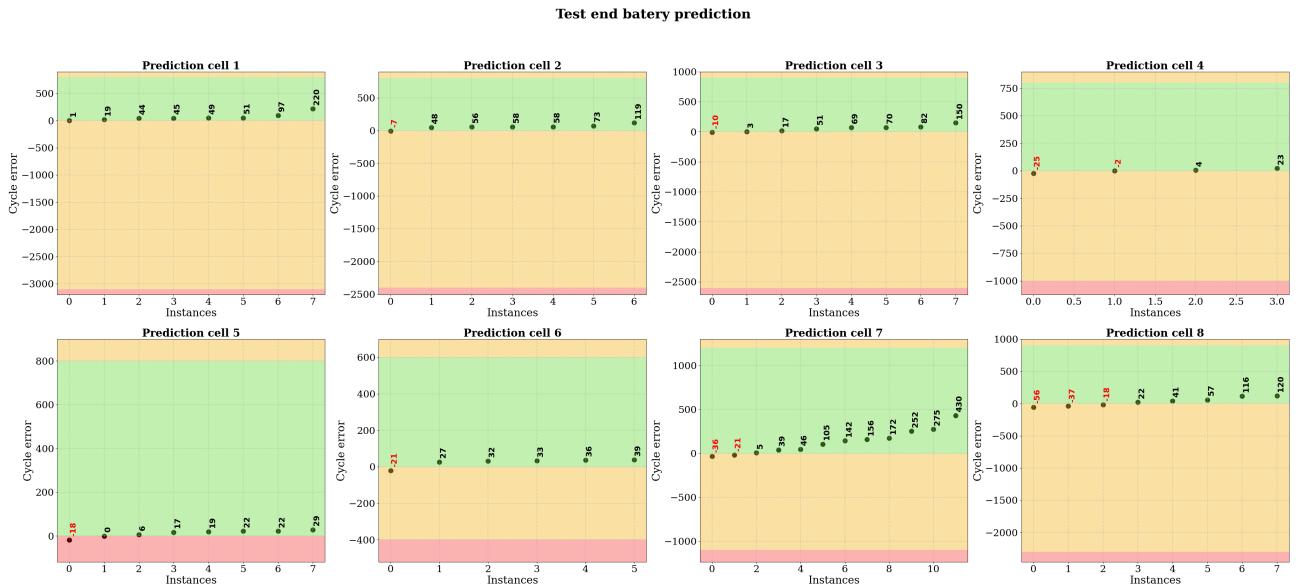


Figure 8. Final test predictions, representing the RUL predicted for each cell using the Bidirectional LSTM and GANs. In red instances with excess of predicted cycles.

improved performance and accuracy in predicting battery degradation.

In summary, the analysis leads to the following key conclusions. Firstly, the utilization of synthetic data has significantly accelerated the training of the Recurrent Neural Network (RNN), enabling upsampling of the training dataset and generating new scenarios within the data. This has proven to be beneficial for model performance.

Secondly, the developed stratification strategy has played a crucial role in facilitating the RNN's learning process by encompassing a wide range of scenarios. The diverse behaviors exhibited by each battery have contributed to a more comprehensive understanding of the overall system dynamics.

Lastly, the implementation of the custom loss function has had a positive impact by effectively penalizing predictions that would be estimated as unaccept-

able in terms of battery performance. This tailored loss function enhanced the models' ability to make accurate predictions that align with the expected behavior of the batteries.

5.2 Future work

As future lines, first, it could be of interest to investigate the interpretability of the deep learning models applied in order to better understand the behavior of the model and improve its predictions. Several methodologies have emerged in recent years, which aim to explain the reason behind the outcomes of complex algorithms. [32]

Additionally, the implementation of new architectures and layer configurations is also not ruled out. The current limitation in equipment has conditioned the complexity of the algorithm architectures proposed. Increasing the number of recurrent layers and

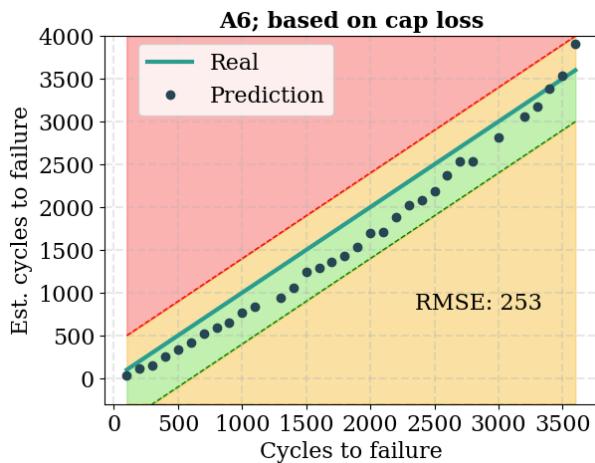


Figure 9. Predictions of the Bidirectional LSTM plus GANs for the sixth battery. All but two of the predictions have been rated as excellent, with two rated as acceptable.

tuning its configuration might have a positive impact on the global performance of the model, as well as trying out new step-batches.

Moreover, it could also be interesting to improve the data augmentation stage. Some different approaches such as LSTM and Variational Autoencoder based approaches (VAE-GANs) have become quite popular in recent years for time-series data generation, so they might improve the generation of new data [33]. It is often believed that the efficiency of data augmentation processes is determined by the improvement of the metric of the task. However, the suitability of the synthetic data generated must be somehow measured in future cases.

Finally, this research has only focused on RNN approaches. So, carrying out experiments with both different RNN approaches and other kind of deep learning algorithms could offer a wider range of possibilities and opportunities in order to solve the problem proposed.

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