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Advanced Lithium-Ion Battery Prognostics: A Comprehensive Review of Machine Learning Approaches for Remaining Useful Life Prediction

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Abstract

The lithium-ion battery (LIB), as one of the main sources for portable power systems, has been increasingly popular owing to its widespread applications in electric vehicles, consumer electronics, aerospace, and renewable energy. Despite their advantages in high energy density and long cycle life, LIBs suffer from degradation over time of aging and cycling, resulting in loss of performance, safety issues, and economic bottlenecks. Predicting their remaining useful life (RUL) is critical for proactive maintenance, cost savings, and prolonging the operational life span. Classical physics-based models face a challenge to capture the complex non-linear degradation patterns of LIBs, which stem from multiple coupled electrochemical processes like solid electrolyte interphase (SEI) formation, lithium plating, mechanical stress, and electrolyte decomposition. These are compounded by external influences such as temperature, depth of discharge, and charge rates. Machine learning (ML) provides an attractive alternative by learning degradation mode from data without using explicit physical equations. Models such as support vector regression (SVR), random forest (RF), Gaussian process regression (GPR), and deep learning models like Long Short-Term Memory (LSTM), convolutional neural network (CNN), and hybrid networks have achieved great success in estimating RUL. The emerging trends are transfer learning, survival analysis, and explainable AI (XAI) for generalization, reliability, and interpretability of the models under a wide diversity of chemistries and real-world conditions. This is all done despite outstanding difficulties such as modeling the capacity recovery, uncertainty quantification, and varying cell form factors. Such frameworks as Battery ML provide a glimpse of how domain-aware engineering is already beginning to integrate with AI, evolving toward intelligent lifecycle management of next-gen battery systems.

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Keywords: Lithium-ion batteries (LIBs), remaining useful life (RUL) prediction, machine learning (ML), battery degradation mechanisms, explainable artificial intelligence (XAI)

INTRODUCTION

This report examines the critical role of lithium-ion batteries (LIBs) in contemporary technology, the inherent challenges associated with their degradation, and the transformative potential of machine learning (ML) to address these issues through remaining useful life (RUL) prediction [1–3].

Significance of LIB and Degradation Challenges

Lithium-ion (Li-ion) batteries are deployed as a key energy storage technology that underpins modern energy services, covering areas that include electric vehicles (EVs), grid-scale storage, aerospace, and consumer products. The high energy density, low self-discharge, and long cycle life of these supercapacitors have made them appeal for a wide application [4–5]. The capability of LIBs to store and then discharge substantial amounts of energy has dramatically changed many facets of society and has worked actively in favor of decreasing CO_2 emissions and improving the handling of energy (Figure 1).

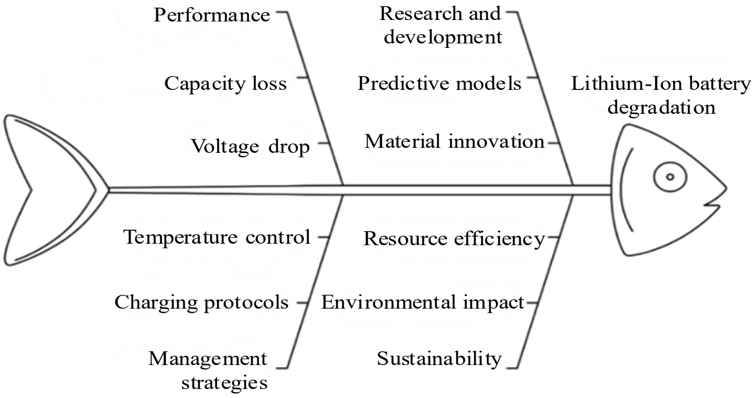

Figure 1. Cause and effect structure of enhancing lithium-ion battery longevity.

Although LIBs exhibit excellent performance, they are inherently prone to aging and degradation during their operation. Aging is characterized by the gradual degeneration of performance parameters, such as capacity fade, power drop, and rise in internal resistance. The widespread battery degradation is a significant challenge for system reliability, operational safety, and economy. This degradation may translate into increased maintenance costs, unplanned outages, and reduced life for battery-reliant systems, which also affect the overall productivity and profit [6–10].

A key observation of battery science is the innate connection between the high-performance features of LIBs and their vulnerability to degradation. The electrochemical processes that LIBs rely on to store and deliver energy most efficiently result in slight, but cumulative degradation of the battery's internal structure as it is charged up and discharged all over again. This implies that factors conferring superior performance simultaneously underlie their loss of sustainability. Accordingly, the removal of degradation in current LIB chemistries is likely insurmountable [11, 12]. This will require the adoption of a new R&D paradigm in which we move away from the "Prevent" mode of thinking about failure, instead focusing on the prediction, monitoring, and control of degradation throughout the battery life cycle. This would be necessary to drive a shift, which is essential for maximizing the usability and lifetime, safety, and economical utilization of battery-based systems (Figure 2).

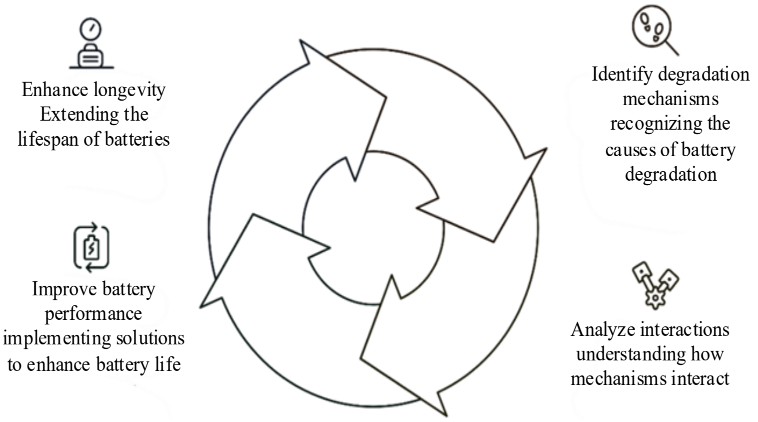

Figure 2. Cycle of lithium-ion battery degradation.

Importance of RUL Prediction in Modern Applications

The concise estimation of the battery's RUL is one of the most essential tasks to improve the maintenance schedule, effectively save operational costs, enhance the security position, and maintain efficient operation properties for many critical applications, such as electric cars and grid energy storage systems. This predictive capability permits a "maintenance before failure" strategy, which can be scheduled at your convenience and will result in no sudden or unplanned downtime. This prolongs the life of battery assets and reduces related risks, turning maintenance from a reactive, expensive task to a scheduled, proactive activity [13–15].

RUL is commonly characterized by the remaining cycles or time until the battery capacity degradation attains a predefined critical level. This threshold is usually approximately 70% or 80% of its initial rated capacity and represents the end-of-life (EOL) of the battery for nearly all applications [16]. The repeated focus in these studies on the fact that RUL directly influences the optimization of maintenance schedules, cost savings, and improvement of safety is a strong indication that even for researchers and experts, there is more to it than just another technical diagnostic tool; it is seen as a strategic enabler to improve economics and safety. It enables a transition from reactive, expensive repairs to scheduled preventive maintenance, which is one of the cornerstones of contemporary industry [17]. This estimates RUL critical for the widespread implementation and maintenance of battery-dependent applications, particularly in the paradigm of Industry 4.0. Supplying actionable intelligence to battery health changes the status of battery management from reactive to strategic, making it a valuable part of an efficient system with economic added value (Figure 3).

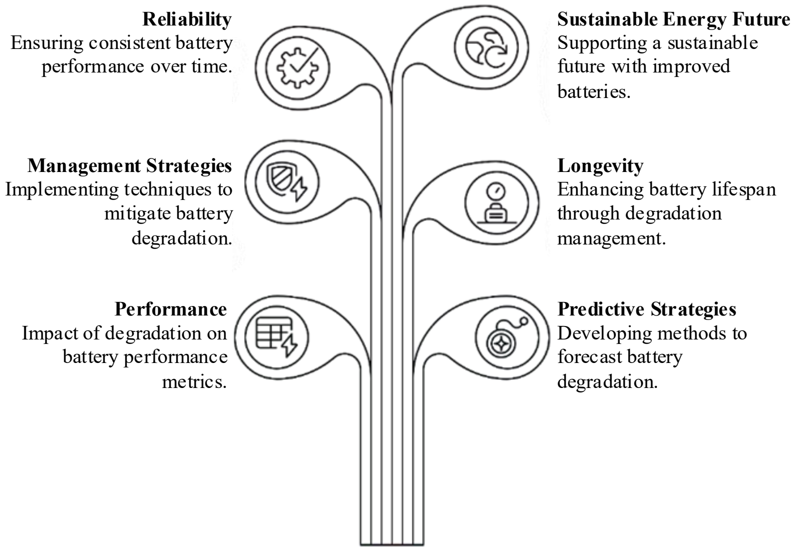

Figure 3. Dimensions of battery degradation.

The Evolving Role of ML in Battery Prognostics

- Model-based methods in recent years, ML approaches have proven to be a powerful, non-intrusive, and computationally efficient form of RUL prediction that can alleviate many of the limitations of traditional model-based methods. Conventional models are prone to sophisticated non-linear degradation behaviors and convoluted intrinsic electrochemical mechanisms of LIBs, leading to inaccurate long-term predictions.
- ML models have an inherent capability to learn complex and non-linear relationships directly from the colossal amounts of operational statistics. This makes them more amenable to manufacturing variations and a range of battery chemistries compared to their physics-based counterparts. A platform, such as BatteryML, is illustrative of this evolution and provides a single, open-source infrastructure for dataset preprocessing, feature creation, and training, not only conventional but also the most advanced ML models [17]. This promotes joint research and accelerates the development of battery prognosis.

- The principal distinction between traditional model-based RUL prediction and ML is the philosophy on which they are based. Generally, conventional techniques may involve a detailed understanding of physical systems and complex electrochemical equations to explicitly describe degradation. However, ML methods do not inherently require the study of intricate internal workings and electrochemical processes but learn patterns from operational data without guidance. This is a fresh perspective from the body of work done before (even in condition-based maintenance), where modeling was explicit and based on first principles, whereas finding patterns is implicit. This fundamental shift offers tremendous opportunities for accelerating battery research because a medical analogy can be drawn to battery development: faster development cycles and the applicability of prognostic models across different batteries. This, in turn, minimizes the dependence on detailed, chemistry-specific mechanistic models that are costly both to set up and to evaluate [18].

FUNDAMENTALS OF LITHIUM-ION BATTERY DEGRADATION

In this section, we address the internal mechanisms and extrinsic factors that contribute to the permanent degradation of LIBs, including structural/chemical changes that can be used as a guide for establishing a degradation model for various battery form factors.

Core Degradation Mechanisms

The degradation of LIBs is a multifaceted and closely related process that occurs within a cell. Key mechanisms are the growth and consumption of the solid electrolyte interphase (SEI) at the anode surface, consuming lithium and electrolyte species, leading to an increased internal resistance and reduced capacity. Lithium plating, which is usually induced by a very high rate of charging or low temperatures, results in metal lithium deposition on the anode, which causes irrecoverable capacity reduction and may lead to short-circuiting [19]. Loss of the active material (LAM) and lithium inventory loss (LLI) also lead to performance decay with electrode degradation and irreversible lithium consumption. Despite the cracking and detachment of electrode materials during expansion–contraction cycles, which increase resistance and hinder ion migration, the mechanical durability of electrodes remains a challenge. Furthermore, the decomposition of the electrolyte at high temperatures or voltages accelerates SEI formation, which then covers the active material. These are interdependent; SEI leads to lithium and electrolyte depletion, increasing the current density, which results in further degradation [20]. This intertwined, non-linear behavior demonstrates that battery degradation is not just a succession of events but rather a synergistic web of reactions. As a result, the precise prediction of degradation and RUL needs sophisticated multiphysics or data-driven ML approaches that can capture these interactions at multiscale multiclass scales (Figure 4).

Key Factors Influencing Degradation

The degradation of the battery is significantly influenced by many extrinsic and operational factors that affect either the rate or the underlying mechanism (Figure 5). Crucial operational parameters are the charge/discharge rate (C-rate) if high C-rates for fast-charging or high-power materials cause degradation by excessive heat development or side reactions such as lithium plating in the case of excessive discharge. Depth of Discharge (DoD) and State of Charge (SoC) histories are important because deeper cycling or more extended high SoC will induce higher mechanical strain, resulting in side reactions that will accelerate capacity loss [21]. Of the environmental considerations, temperature is paramount: extreme heat and cold both weaken SEI stability, change electrolyte dynamics, and hasten chemical breakdown, whereas calendar life degrades with time even in the absence of any use (primarily caused by storage temperature and SoC). Other factors, such as driving conditions, cell balancing, and manufacturing variations, also contribute to shaping degradation behavior. With all these intertwined effects and non-linear couplings, monitoring only the capacity fade is not sufficient for reliable prognostication. Rather, complete information gathering, including thermal, electrical, and contextual information, is required [22]. Therefore, a reliable RUL prediction requires feature-rich, multidimensional datasets and advanced ML models that are able to capture the integrated operating and environment dynamics that drive true battery aging.

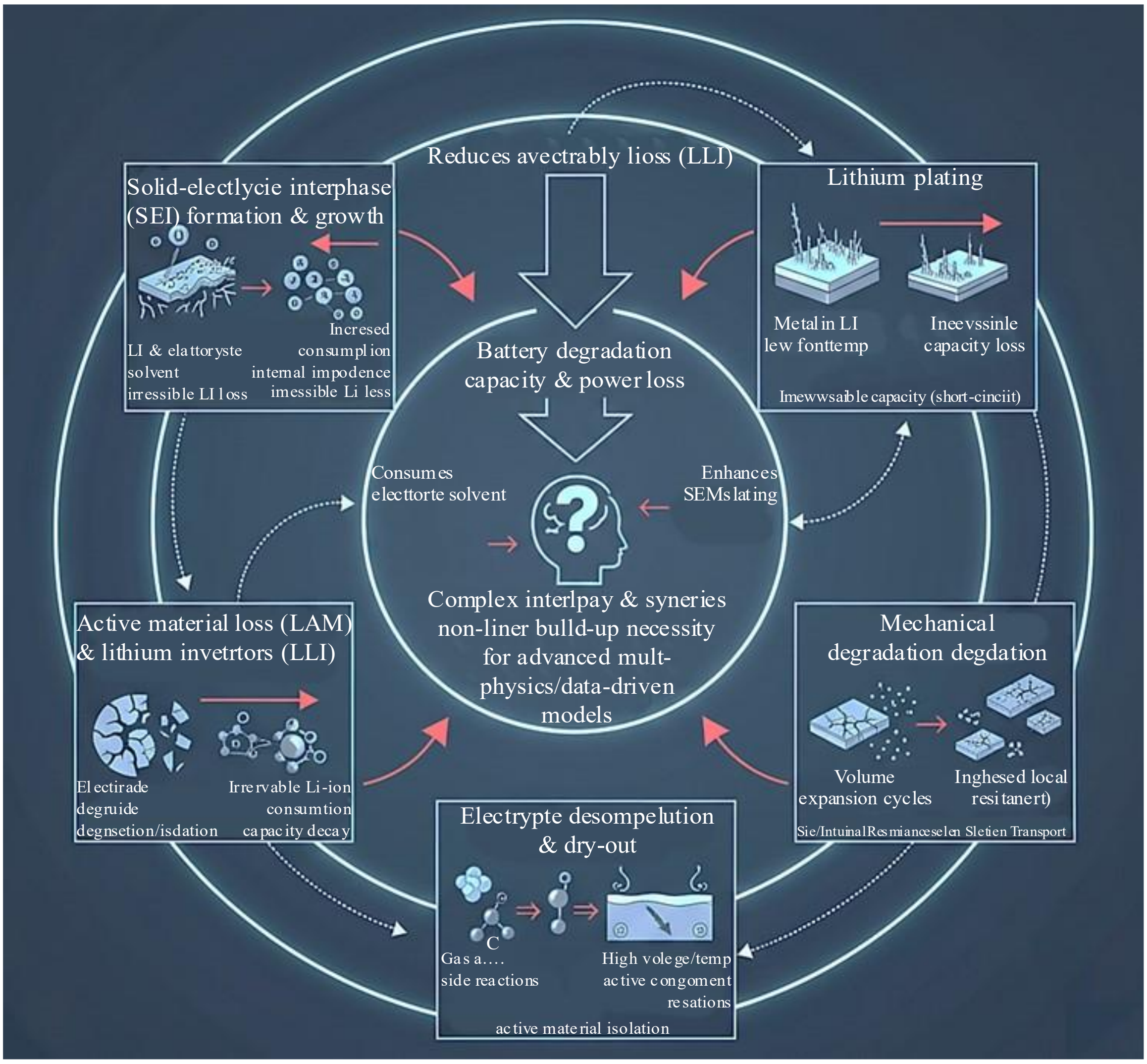

Figure 4. Interconnected battery degradation mechanisms.

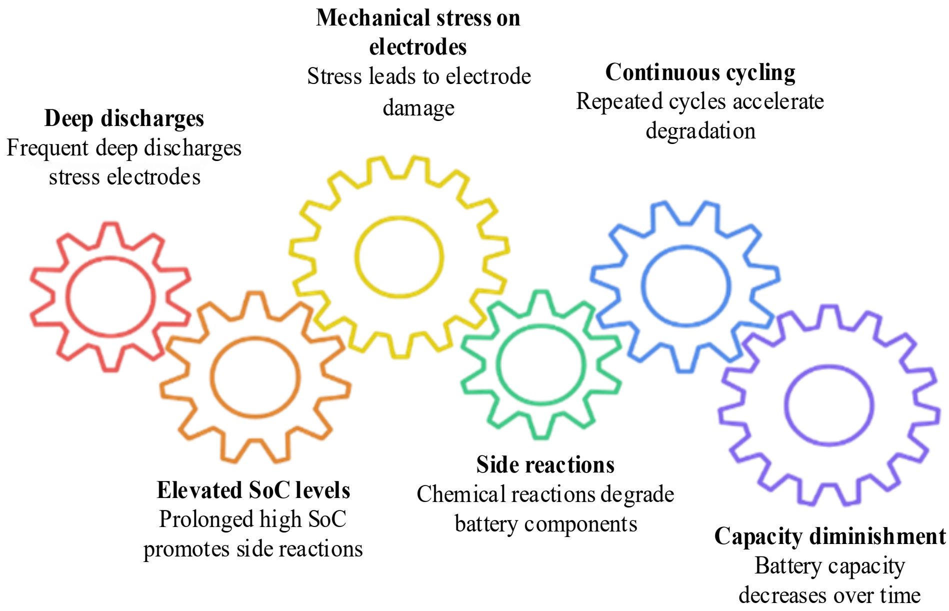

Figure 5. Battery degradation processes.

Influence of Battery Form Factors (Cylindrical, Prismatic, Pouch) on Degradation Pathways

The form factor of the LIB cell, either cylindrical, prismatic, or pouch, largely dictates its structural integrity, thermal behavior, and degradation pathways. Cylindrical cells (18650, 21700, etc.), including Positive Temperature Coefficients (PTCs) and Current Interrupt Devices (CIDs), are housed in tough metal enclosures with superior mechanical strength and inherent safety features. However, they inevitably have a large heat-generation volume and low packing ratio, leading to poor charge-discharge capacities in the frequent formation of SEI, lithium plating, and electrolyte oxidation layers [23, 24]. The prismatic cell has a box-like structure and metallic enclosure, which can facilitate space saving, stacking arrangement, and cooling enhancement of cells. However, the internal pressure may not be uniform, particles are broken and crushed, and lithium ions are trapped, resulting in weak long-term reliability. Pouch cells are lightweight and flexible, providing design flexibility and better heat dissipation from a higher surface-area-to-volume ratio, both of which make pouches an excellent choice, but they consist of no mechanical protective attributes or inherent safety features. This makes them more sensitive to swelling, electrode delamination, and mechanical deformation, which reduces the performance and life of batteries [25–27]. In the final analysis, the physical geometry of the individual form factors determined the thermal and mechanical degradation modes. Gaining insight into such relationships is important for choosing a suitable type of cell for a given application, as well as to develop form factor-aware prognostic models that can accurately predict the RUL across various operational conditions (Table 1).

Data Acquisition, Preprocessing, and Feature Engineering for ML-Based Prognostics

Data quality plays a critical role in machine learning-based diagnostic and prognostic models. These results indicate that correct database construction, preprocessing, and characteristic extraction are critical elements for battery health and RUL estimation [28].

Data Collection

Battery training data are commonly obtained from three sources (Figure 6). One is the laboratory discharge data (i.e., constant current-constant voltage (CC-CV), hybrid pulse power characterization (HPPC), and electrochemical impedance spectroscopy (EIS) tests) that can be carried out to enable controlled conditions to investigate the degradation characteristics at different current rates, voltage thresholds, and temperatures. Second, open-source datasets made available by organizations such as CALCE, NASA Ames, MATR, HUST, and Rheinisch-Westfälische Technische Hochschule (RWTH) provide real-life run-to-failure time-series data necessary for developing and testing prognostic algorithms. Third, the traces collected with simulation tools such as ADVISOR2002 and PyBaMM can be used to create simulated datasets for diverse operating conditions, aging mock-ups, backing up experimental data, and covering areas that are difficult to test. In such sources, important battery parameters (voltage, current, temperature, and capacity impedance) are captured under various operating conditions and applied to create accurate and cross-applicable RUL models [29–31].

Data Preprocessing and Feature Engineering

Preprocessing: changes the raw data to a usable structure in the model through cleaning, normalization, and feature creation. Data cleaning removes outliers, imputes missing entries, and reduces sensor noise. Standardization guarantees that all parameters are on the same scale, for example, of the order of magnitude: voltage (2.5–4.2 V), current (−4 to + 2 A), or temperature (0 Â ±45 Â °C), and a variety of data smoothing and denoising techniques such as median filtering or wavelet decomposition may improve the reliability and quality of data. Platforms such as Battery ML employ a canonical data structure (e.g., Battery Data) to normalize diverse datasets. Simulations to generate synthetic data have been widely used as the training sample is always small, and this method can simulate degradation conditions [32–37].

Table 1. Battery cell comparison.

Characteristic	**Cylindrical**	**Prismatic**	**Pouch**
Structure	Metal casing	Rectangular casing	Foil casing
Thermal Management	Good	Moderate	Limited
Degradation Modes	Stress, runaway	Swelling, leakage	Puncture, runaway
Pros	High density	Space-efficient	Lightweight
Cons	Bulky	Expensive	Vulnerable
Typical Applications	Power tools	Consumer electronics	Smartphones

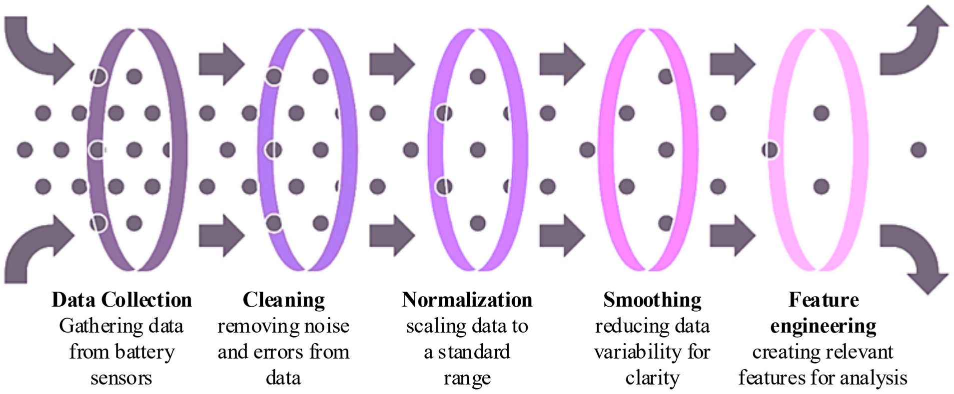

Figure 6. Data processing funnel.

Feature Engineering focuses on extracting informative indicators that describe battery performance and aging. Intra-cycle values (like QdLinear, Coulombic efficiency, or internal resistance) reflect the behavior during charge/discharge. History-based information (e.g., rate of degradation, charging duration, and temperature) characterizes the long-term patterns across cycles. When direct capacity data are missing, aging is quantified using health indicators (HIs) computed from voltage, current, and temperature information. To model time-to-failure, the observations are rephrased as the number of cycles or times before a battery exceeds a failure threshold and account for censored data from experiments that have not terminated [38]. Finally, we apply dimensionality reduction methods, such as principal component analysis (PCA), to select the most informative features for increased computational speed and model accuracy.

ML Models for RUL Prediction

ML algorithms are powerful for predicting the RUL of batteries, partially because of their ability to encode complex and non-linear degradation, rather than an explicit requirement for physical models. Conventional ML models such as support vector regression (SVR), RF, and ensemble methods such as XGBoost, LightGBM, and CatBoost have shown a good balance between model performance and interpretability. SVR can deal robustly with noisy data via kernel-based transformations, which implies its suitability for real-time RUL prediction (Figure 7). RF and ensemble methods integrate multiple decision trees to increase accuracy, robustness, and generalization, and reduce overfitting. Gaussian process regression (GPR) yields probabilistic predictions accompanied by confidence intervals, which are beneficial under unknown or uncertain operating conditions but have a high computational cost, especially for large datasets. Linear regression (LR), though simple, is still powerful at capturing linear behaviors in degradation (especially with cycle count used as features) and can provide interpretable and reliable results for some applications [39].

Deep Learning Models

Deep learning (DL) models emerge as powerful tools for predicting the RUL of batteries because they can learn complex patterns and long-range temporal dependencies of time-series data. Long Short-Term Memory (LSTM) and its variations (i.e., bi-LSTM) are good at modeling the temporal degradation pattern by sequentially learning from sequential data, whereas CNNs directly extract spatial features without interactive manual feature extraction. Hybrid models such as CNN-LSTM, attention-LSTM, and their variants or leans [24] are often fused with Neural Ordinary Differential Equations (ODEs) to combine the power of local learning and long-term temporal modeling for continuous degradation dynamics prediction. The DLinear model is a lightweight and interpretable model for capturing trends and seasonality and can perform better than more complicated networks. In addition, deep survival models such as DeepHit and Multi-Task Logistic Regression MTLR, coupled with survival analysis frameworks (e.g., Cox model), yield probabilistic RUL predictions and uncertainty estimation by characterizing battery failure as a time-varying process (Figure 8).

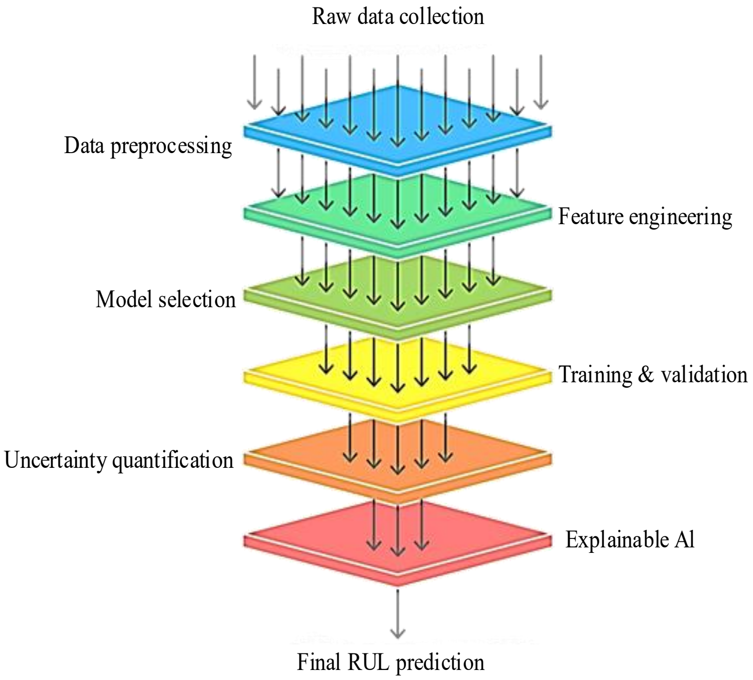

Figure 7. RUL prediction workflow.

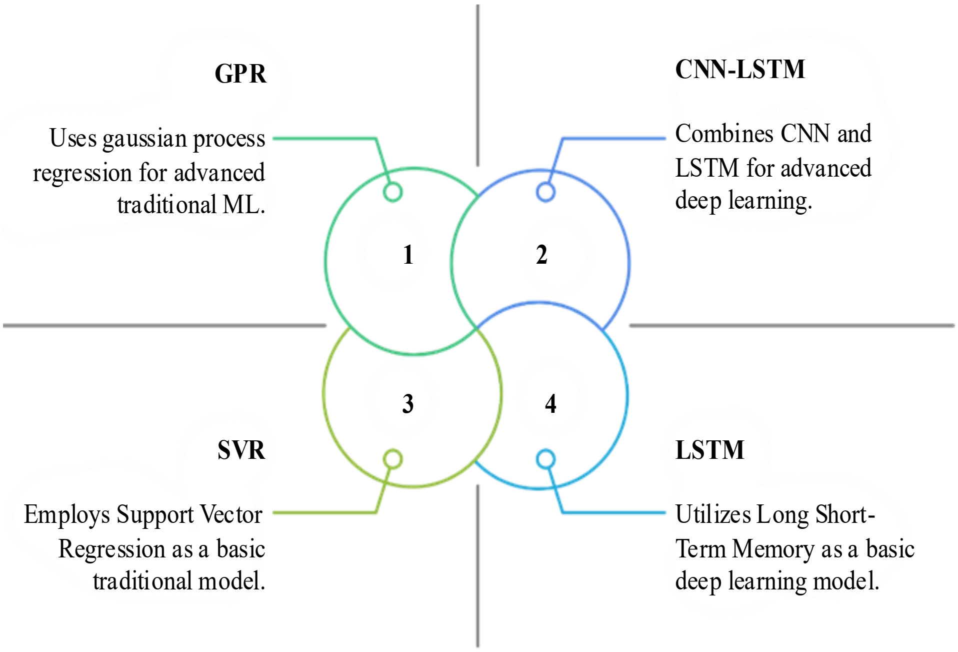

Figure 8. ML models in RUL prediction.

Uncertainty Quantification in RUL Prediction

Uncertainty Quantification (UQ) is gaining importance in the context of RUL prediction because of its critical role in reliable estimates, particularly for safety-critical applications. It is an indicative source of the confidence level in making predictions, which is essential for decision making (Table 2).

Types of Uncertainty

Aleatoric Uncertainty: This corresponds to natural randomness and variability in the system, for example, owing to sensor noise or state-transition perturbations. It is incompressible, cannot be overcome by adding more data, and is key to understanding the quality of predictions in noisy or unstable worlds.

Epistemic Uncertainty: It is caused by ignorance or incomplete knowledge of the system or model. Appropriate values of either drive the term to zero, or it may be in any range if more information, a better model and algorithm, or experiment/data are/is available.

Evidential deep learning (EDL): EDL is a potential solution for simultaneously learning RUL and mapping aleatoric and epistemic uncertainties. It fits a neural network to generate higher-order evidence distribution hyperparameters, which enable the representation of deeper levels of uncertainty without performing any sampling. The EDL is robust to noise levels because it can measure both forms of uncertainties [40].

Probabilistic Models: GPR, as mentioned earlier, gives confidence intervals and, hence, measures uncertainty directly along with predictions. Other probabilistic methods, such as some approaches, have also been used to estimate uncertainty in DL models.

Addressing Capacity Regeneration

Capacity recovery is such a phenomenon that during resting, the battery's capacity seems to be partially recovered, and this affects the modeling of the degradation trend, which makes RUL prediction complex. To counteract this effect, ML-based approaches have been developed.

Signal Decomposition Technologies

Techniques such as wavelet decomposition technology (WDT) and complete ensemble empirical mode decomposition with adaptive noise (CEEMDAN) are applied to decompose the global degradation trend from local regeneration phenomena in the battery capacity series. This enables the model to learn both the long-term and short-term recovery effects.

Hybrid Models

Integration of signal decomposition (FFT) and neural networks (e.g., NARNN, LSTM) provides accurate predictions for both parts, from which they are summed to obtain the RUL prediction. Some

Table 2. ML Models categories by complexity in RUL prediction

Complexity category	ML models for RUL prediction	Characteristics/notes on complexity
Low Complexity	Gaussian process regression (GPR), support vector regression (SVR), linear/polynomial regression, K-nearest neighbors (KNN), decision tree, Naïve Bayes	Simple mathematical/statistical basis. Fast training and prediction. Good for initial analysis or when data is limited. May struggle to capture highly non-linear degradation trends.
Medium Complexity	Random forest (RF), eXtreme gradient boosting (XGBoost), LightGBM, gradient boosting (GB), multi-layer perceptron (MLP)	Ensemble methods (RF, XGBoost, etc.) combine multiple simple models for higher accuracy and robustness. MLP is a basic neural network. Generally, higher accuracy than low complexity models, but require more computational power.
High Complexity (deep learning)	Long Short-Term Memory (LSTM), gated recurrent unit (GRU), bidirectional LSTM (Bi-LSTM), attention-LSTM, deep neural networks (DNN), auto-encoders	Designed to automatically learn complex, long-term temporal dependencies in time-series data (like capacity fade). High computational cost and large data requirement for training, but often achieve the highest prediction accuracy and generalizability for RUL.

approaches have employed modified predicted HIs with added Gaussian non-white noise to simulate and evaluate capacity regeneration within the prediction confidence bands.

Explainable AI (XAI) in Battery Prognostics

Explainable AI (XAI) is an approach to deal with the “black box” problem in DL, and it aims to gain transparency and interpretability, which are important for safety-critical applications such as battery management systems (BMS). Model explanation enables trust in predictions, debugging, validation of outputs, and testing for potential bias or errors from technical applications.

Key techniques involve SHapley Additive exPlanations (SHAP), which calculate the importance of each feature via game-theoretic Shapley values and depict variables such as temperature, cycle index, voltage, and current impact battery degradation. Although SHAP provides both detailed and global interpretations, it can be computationally expensive for high-dimensional data. Attention models provide interpretability to sequence models by revealing which parts of the historical battery data are most relevant when predicting RUL, thus connecting past behavior to expected life [41]. Moreover, inherently interpretable models, such as Dlinear, come with explainability out of the box via their linear structure and parameter weights in terms of feature importance and behavior.

Transfer Learning for Limited Data Scenarios and New Battery Chemistries/Form Factors

Transfer learning (TL) is an influential approach for improving the generalization performance of ML models because it transfers learned knowledge from one domain/dataset to a target domain with limited data. This is especially beneficial in the battery prognostics case, where collecting large and diverse datasets for each new chemistry or form factor can be expensive and time-consuming (Figure 9).

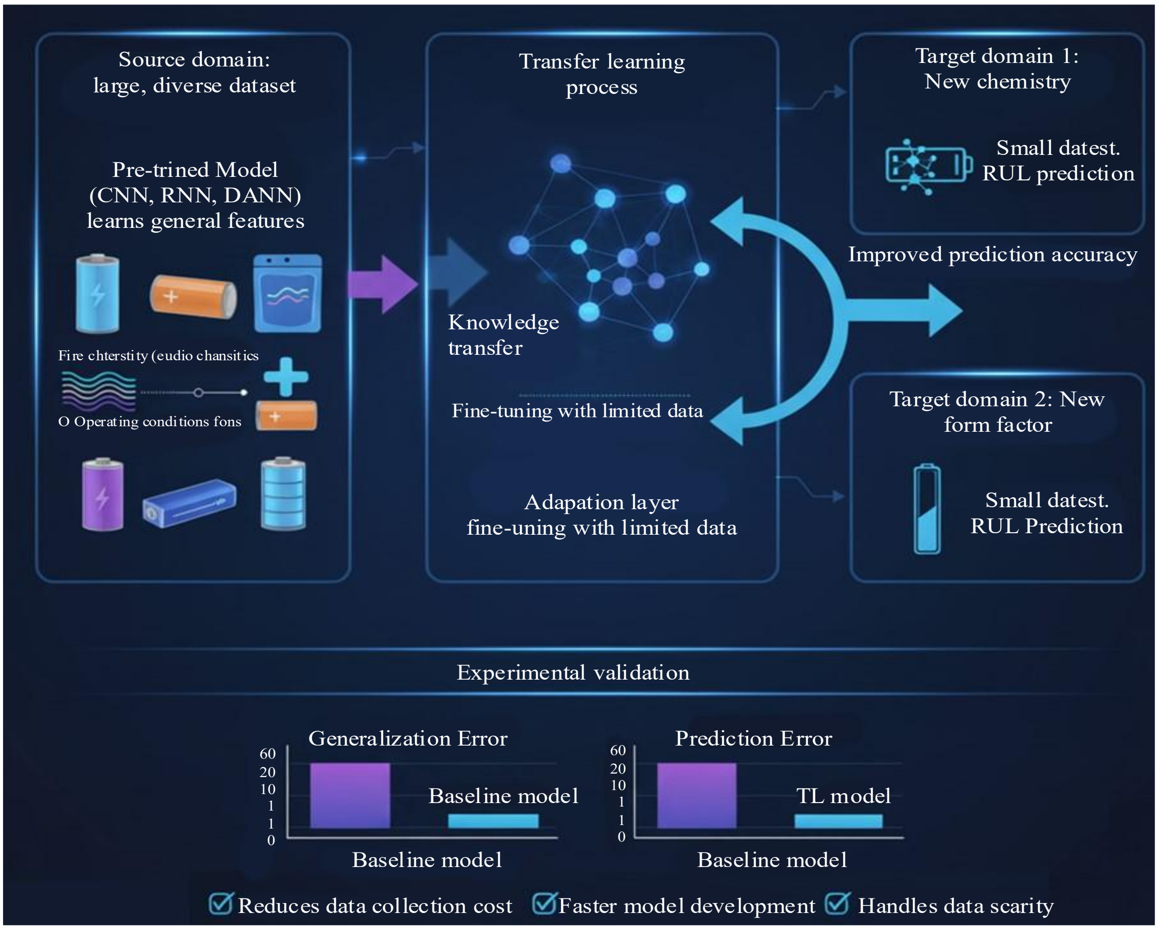

Figure 9. Transfer learning for battery prognosis.

Dealing with limited data: TL achieves good RUL prediction results even on small or mismatched target datasets under operating conditions compared to the training dataset. By transferring knowledge by pre-training models on large datasets and subsequently fine-tuning them with a small amount of new data, TL dramatically improves the prediction models.

Cross-domain generalization: TL helps to use models built from one battery chemistry/form factor on another form factor/chemistry, enabling the transfer of robustness and reducing the requirement for significantly new experimental data. Domain adaptation methods, for example, those based on domain-adversarial neural networks (DANN) or maximum mean discrepancy (MMD), enable the learning of domain-invariant features, thereby improving generalization towards unseen data distributions.

Experimental validation: The studies show that TL-based methods can outperform or have the same prediction performance as the models trained on one battery and can be applied to other batteries with similar operating conditions. This also leads to a notable drop in the generalization and prediction errors compared to the baseline models.

MODEL VALIDATION AND PERFORMANCE METRICS

Validation is the final step to ensure that such ML-based RUL predictive models are robust, accurate, and generalizable. Commonly used validation methods and performance indicators for battery prognostics are described in this section [42].

Validation Techniques

Cross-validation (CV): CV methods are essential for evaluating the robustness and generalization of ML models, particularly for predictive time-series data.

Time-Series Cross-Validation: This technique uses test sets composed of single observations, along with training sets containing only data prior to each given test set. This “rolling forecasting origin” process prevents future observations from affecting the forecast and allows for realistic validation of the model’s accuracy when forecasting in a sequential manner on out-of-sample data.

Leave-One-Out/Leave-One-Triplicate-Out: This approach (applicable to datasets derived from several cells or replicates) consists of training the model on all but one (or one triplicate) cell and then testing it on the removed cell. This tested how well the model could be generalized to new manufacturers or cycling conditions.

Train-Test Split: A basic validation method that divides the data into training and testing sets (e.g., 80-20%). The model was trained on the training set and tested on the test set to evaluate its generalization ability.

Run-to-Failure Trajectory Analysis: Models are confronted with run-to-failure time-series data, and the experiments terminate when the battery accumulates an EOL threshold value (e.g., a 30% or 20% decrease in rated capacity). This makes the prospective testing of prognostic algorithms feasible for actual EOL.

Comparison to Baselines and State-of-the-Art: To evaluate the efficacy of a model, we benchmarked it against existing baseline models (e.g., classical ML or simpler DL architectures) as well as other prior high-performance methods in the literature.

Performance Metrics

There are several quantitative metrics used for the evaluation of RUL prediction models, including:

Error Metrics

RMSE (root mean squared error): a standard metric that averages the magnitude of errors. It depends on large errors and is the most common measure of accuracy.

Mean absolute error (MAE): Average absolute error between predicted and true values. It is less sensitive to outlying scores than the RMSE.

MAPE (mean absolute percentage error): Scale-dependent, percentage type error; range is 0 to ∞; lower values are better.

Goodness of Fit Metrics

R-squared (R^2): This value indicates the amount of variation predictable based on the independent variable. Larger R^2 values indicated a better fit of the model to the data.

Prognostic-Specific Metrics

Remaining useful life error: The predicted RUL and its actual value are typically operating cycles or time.

C-index: A concordance index used in survival analysis to describe the extent of agreement between predicted risk scores and the actual time until events.

IBS (integrated brier score): An estimator from survival analysis that measures the calibration quality of survival probability predictions as a function of time, with lower scores indicating better calibration.

Confidence Intervals (CIs): CIs allow probabilistic models to propagate the uncertainty of prediction into an interval within which one can expect the actual RUL.

Computational efficiency: The training and prediction time must be minimal, and in real-time applications of BMS, this is more exigent. Computational costs of models such as RF with extra tree regressors and LR [43].

RESULT AND DISCUSSIONS

Figure 10 shows the Challenges and Solutions of the LIB Prognostics. Table 3 illustrates the comparison between ML and DL models for LIB.

Table 3. Comparison of ML and DL models for lithium-ion battery RUL Prediction.

Approach / Model Type	Significant Features	Limitations	Applications / Remarks
Support vector regression (SVR)	• Handles non-linear degradation via kernel functions. • Robust to noise and small datasets. • Suitable for real-time on-board estimation.	• Sensitive to kernel choice • Limited scalability with large datasets	• On-board battery management systems (BMS) • Compact EV modules
Random forest (RF) and ensemble models (XGBoost, LightGBM, CatBoost)	• Captures non-linear, temporal patterns. • High accuracy, low overfitting. • Feature importance available.	• Computationally heavy for very large datasets • Limited interpretability	• EV fleet RUL monitoring • Industrial-scale energy storage
Gaussian process regression (GPR)	• Probabilistic model with confidence bounds • Handles uncertainty (Aleatoric + Epistemic).	• Computationally expensive ($O(n^3)$) • Poor scalability for large datasets	• Laboratory validation and small dataset modeling • Uncertainty-aware RUL estimation
Linear regression (LR)	• Simple, interpretable, low computational cost • Works well with engineered degradation features.	• Assumes linearity • Poor fit for complex, non-linear degradation	• Baseline prediction model • Quick RUL estimation with minimal data
Long short-term memory (LSTM)	• Captures long-term dependencies in time-series	• Requires large data and compute	• EVs and grid batteries under continuous

	• Models sequential degradation patterns effectively.	• Opaque model (less interpretable)	monitoring • Predictive maintenance scheduling
Convolutional neural network (CNN)	• Learns spatial patterns in raw data • Reduces need for manual feature engineering.	• Limited temporal understanding alone • Needs hybridization with RNN/LSTM	• Used in CNN-LSTM hybrids for degradation signal extraction
Hybrid models (CNN-LSTM, attention-lstm, NODE, DLinear)	• Combine spatial-temporal learning • DLinear adds interpretability and efficiency • NODE models continuous degradation dynamics.	• Complex to train and tune • High data and computing requirements	• Advanced prognostic systems in aerospace and EVs • Long cycle industrial batteries
Survival analysis (DeepHit, MTLR, Cox models)	• Models probabilistic "time-to-failure" events. • Handles censored data. • Provides reliability estimates.	• Needs specialized data (failure-labelled) • Difficult to interpret in high dimensions	• Safety-critical systems (aerospace, defense) • Probabilistic RUL assessment
Evidential deep learning (EDL)	• Quantifies both aleatoric and epistemic uncertainty. • Robust to sensor noise. • No need for sampling.	• Complex mathematical framework • Requires careful training and stability	• Battery Health Management under uncertain conditions
Transfer learning (TL)	• Enables cross-chemistry or cross-form factor prediction. • Effective in limited data scenarios. • Enhances model generalization.	• Risk of negative transfer (mismatch between domains)	• New battery chemistries • Accelerates RUL modeling for novel cells
Signal decomposition + ML (e.g., WDT, CEEMDAN + LSTM)	• Separates global degradation from local capacity recovery • Improves prediction accuracy.	• Preprocessing intensive • Not real-time friendly	• Batteries showing capacity regeneration behavior
Explainable AI (SHAP, attention mechanisms)	• Improves the interpretability of ML models. • Identifies key degradation drivers (SoC, temperature, cycle index).	• Computationally expensive for deep models	• Regulatory and safety-critical applications • R&D for feature attribution in degradation

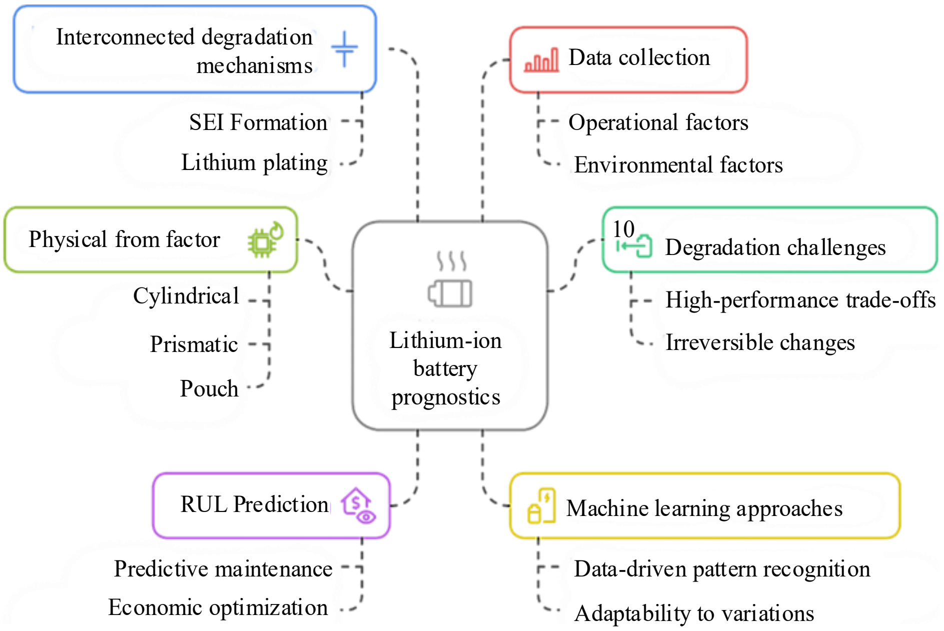

Figure 10. Lithium-ion battery prognostics: challenges and solutions.

CONCLUSIONS

Data-Driven and Domain Knowledge Integration

ML is revolutionary in the RUL prediction of LIB, which can reveal data-driven insights into rather obscure degradation mechanisms. However, including domain knowledge feature engineering in combination with ML-based models is of paramount importance in maintaining physical consistency and interpretability. This mixture addresses the distance between theory and practical applications.

Positives and Negatives of ML Models

Classical algorithms, including support vector regression (SVR), RF, and GPR, can interpret small datasets well, and DL models such as LSTM and CNN are suitable for modeling long-term and non-linear dependencies in large-scale data. The best choice of model is determined by a trade-off between prediction performance, interpretability, and computational time.

Role of Hybrid and Explainable Models

Contemporary research has led to a new paradigm that favors hybrid architectures, such as CNN-LSTM [vc_cnnlstm2], attention-LSTM, and DLinear [dlinear], which take advantage of both temporal and spatial learning. The use of XAI techniques such as SHAP and attention mechanisms can enhance transparency, model validation, and trust, in particular for safety-critical applications such as EVs or aerospace systems.

Dealing with Uncertainty and Capacity Rejuvenation

Predicting future RUL with confidence must include the UQ and consider capacity rebound effects on degradation. Ways such as EDL and signal decomposition methods (WDT, CEEMDAN) enhance the robustness of the model to recognize short-term recovery and long-term degradation events, which is helpful for the prediction of real-world BMS.

Future of Battery Prognostics

The next-gen of LIB prognostics is in TL, physics-informed neural networks, and uncertainty-attentive AI architectures. These methods will allow cross-chemistry generalization and adaptive learning in a scalable manner towards new battery types or form factors. Creating interpretable, data-efficient, and scalable ML systems is essential for realizing safe and sustainable next-generation energy storage technologies.

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