Proceedings Paper:
Liu, K, Yang, Z, Wang, H et al. (2021) Classifications of Lithium-Ion Battery Electrode Property Based on Support Vector Machine with Various Kernels. In: Recent Advances in Sustainable Energy and Intelligent Systems: 7th International Conference on Life System Modeling and Simulation, LSMS 2021 and 7th International Conference on Intelligent Computing for Sustainable Energy and Environment, ICSEE 2021, Han. 7th International Conference on Life System Modeling and Simulation, LSMS 2021 and 7th International Conference on Intelligent Computing for Sustainable Energy and Environment, ICSEE 2021, 30 Oct - 01 Nov 2021, Hangzhou, China. Springer, Singapore, pp. 23-34. ISBN: 978-981-16-7209-5. ISSN: 1865-0929.

https://doi.org/10.1007/978-981-16-7210-1_3

Lithium-ion Battery Electrode Property Classifications for Smarter Manufacturing

Kailong Liu[1], Zhile Yang[2*], Haikuan Wang[3], and Kang Li

[1] WMG, University of Warwick, Coventry, CV4 7AL, UK
[2] Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, 518055, PR China
[3] Shanghai Key Laboratory of Power Station Automation Technology, School of Mechatronic Engineering and Automation, Shanghai University, Shanghai 200072, PR China
[4] School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, U.K

Abstract. Manufacturing chain of lithium-ion batteries belongs to a significantly complex process with many coupled product parameters and intermediate products. To well monitor and optimize battery manufacturing process, it is vital to design a data-driven approach for effectively modelling and classifying the product properties within this complicated production chain. In this paper, a support vector machine (SVM)-based framework, through using four various and powerful kernels including linear kernel, quadratic kernel, cubic kernel and Gaussian kernel, is proposed to well classify the electrode mass loading property of battery. The effects of four crucial variables including three product features from mixing step and one product parameter from coating step on the electrode property classification are also investigated. Comparative results illustrate that electrode mass loading can be effectively classified by the designed SVM framework while Gaussian kernel-based SVM achieves the best classification for all labelled classes. This is the first time to systematically evaluate and compare the performance of different kernel-based SVMs on the battery electrode property classification. Due to data-driven nature, the proposed SVM-based framework can be easily extended to classify other product properties and analyze other variables in battery production domain.

Keywords: Lithium-ion battery, Battery production chain, Support vector machine, Kernel functions, Electrode property classifications.

1 Introduction

Lithium-ion (Li-ion) batteries have been widely utilized as main power source for sustainable energy applications such as smart grids, electrical vehicles and electrical trains, owing to their competitive properties such as high energy density and low self-discharge rate [1]. Due to the battery performance would be highly and directly affected by the related manufacturing processes, an effective production chain that can monitor and analyze battery intermediate product properties is thus vital for boosting the development of Li-ion batteries [2].

However, due to the complexity of containing lots of intermediate processes, numerous variables would be generated in battery production chain. These variables would highly affect the properties of intermediate products, further playing a key role in determining the final battery performance. Therefore, it is crucial to design suitable solutions for better investigating the effects of intermediate product variables (IPVs) on the classification performance of battery product properties.

With the rapid developments of machine learning (ML) algorithms, data-driven approaches are becoming the powerful tools for handling lots of issues within battery managements [3]. To date, numerous data-driven methods have been effectively adopted to estimate dynamics states [4,5], forecast service lifetime [6,7], achieve charging managements [8,9] and energy managements [10,11] of batteries. Overall, reliable analyses can be done by well designing data-driven solutions in battery management domain. However, the analyses of battery manufacturing are still mainly obtained by expert knowledge as well as trial and error methods. It should be known that battery production will also generate a large number of related data, deriving suitable data-driven models to analyze these data should be also considered as a promising way to achieve battery smarter manufacturing.

In comparison with battery managements, fewer attempts have been done so far to derive advanced machine-learning strategies in battery production chain [12]. Among many corresponding themes (process monitoring and adjustments) of battery manufacturing, deriving suitable data-driven model to predict or classify the properties of battery intermediate products is a hot research topic. For examples, a data-driven approach was proposed in [13] to determine the internal parameters for quality controls in battery production. Based upon the cross-industry standard process, Schnell et al. [14] designed linear and neural network (NN) models to forest the product properties of battery manufacturing. Turetskyy et al. [15] proposed the decision tree based models to conduct feature selections and predict the maximal capacity of battery production. In [16], the dependencies of three parameters from mixing step within battery production chain are mainly analyzed by the 2D graphs from a SVM and experimental data. For the aforementioned researches, some common ML algorithms such as SVM has presented powerful potentials to derive suitable models for classifying the properties of battery production. However, many works mainly focus on simply using a common ML algorithm without in-depth investigating its performance in battery production domain. It should be known that the kernel function plays an important role in SVM and also needs to be carefully selected for solving battery manufacturing issues. Therefore, how to design a suitable kernel within SVM to not only achieve acceptable classification accuracy but also present high generalization ability of battery production is still a key but challenging issue.

According to the above discussions, driven by the purpose to effectively classify the product properties of battery production chain, a kernel-based SVM framework is designed in this study. Specifically, after well labelling electrode mass loading into four classes, four crucial variables including three product features from mixing step and one product parameter from coating step are selected as the inputs of SVM to investigate their effects on the classifications of battery electrode mass loading. Instead of simply using a linear kernel, other three powerful kernels including quadratic kernel, cubic kernel and Gaussian kernel are also coupled within SVM for achieving better classification performance. This is the first time to systematically evaluate and compare the classifications of various kernel-based SVMs on the battery electrode property. Experimental results from confusion matrix and ROC curve illustrate the effectiveness of this SVM-based framework, paving a promising way to better analyze and classify other product properties of battery production domain.

2 Key steps in battery electrode manufacturing

The electrode manufacturing of Li-ion batteries belongs to a highly complicated chain which involves many disciplines such as electrical, chemical, and mechanical engineering. Fig. 1 systematically illustrates several key steps in electrode manufacturing.

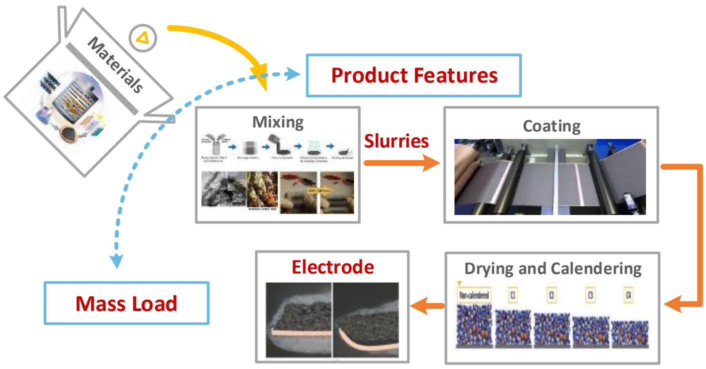

Fig. 1. Key steps in battery electrode manufacturing.

According to Fig. 1, the battery electrode manufacturing chain mainly contains mixing, coating, drying and calendaring steps. In the mixing step, the slurries of both anode and cathode would be produced through mixing the active materials (graphite and Li-NCM-Oxide), the conductive additives (carbon black), the solvent (NMP) and the binder (PVDF) within a soft blender. Then the well-mixed slurries will be coated into a mental foil (generally copper for anode and aluminium for cathode) by the coating machine, followed by a drying process to dry the coating product through using built-in ovens. Finally, the electrodes can be obtained after the calendaring process. It should be known that a large number of variables and parameters can be generated during such complex electrode production chain. The product features and parameters from key steps such as mixing and coating are significantly important for the electrode properties, which would further affect the final performance of battery products and must be carefully analyzed.

In light of this, some representative product features from mixing as well as coating steps are selected to develop suitable kernel-based SVM for classifying the electrode properties in this study. To be specific, four product features or parameters including the active material mass content (AMMS), solid-to-liquid ratio (STOLR), viscosity and comma gap (CG) are utilized to build the SVM models for investigating their effects on the classification results of one battery electrode property named electrode mass loading (electrode mass per unit area). In theory, STOLR is the mass ratio between slurry solid (active material, conductive carbon as well as binder) and mass (solid component as well as solvent). Viscosity impacts the shear rate within coating step. CG is the gap between comma roll and coating roll within a coater. According to these selected product variables and electrode property, the original manufacturing data from Laboratoire de Reactivite et Chimie des Solides (LRCS) are explored. The effectiveness of these data has been proven in [16], which would not be repeated here due to space limitation. For these data, because eight same samples of product features are utilized to obtain one mass loading of battery electrode, the original data would be first compressed to 82 samples through averaging them with the same observations. Then the electrode mass loading would be classified into four grades with the labels as Grade 1, Grade 2, Grade 3 and Grade 4, respectively. The detailed rules of setting these labels are described in Table 1.

Table 1. Detailed rules of setting labels for battery electrode mass loading.

Label setting	***Electrode mass loading (EML)[mg/cm²]***
Grade 1	$EML \leq 18$
Grade 2	$18 < EML \leq 30$
Grade 3	$30 < EML \leq 42$
Grade 4	$42 < EML$

Based upon these selected product variables and predefined class labels, the SVM model could be built to evaluate and quantify the effects of various kernels on the classification performance of battery electrode mass loading.

3 Technology

In this section, the fundamental of SVM classification is first presented, followed by the descriptions of four various kernel functions. Then the indicators to evaluate the classification performance are also described.

3.1 Support Vector Machine Classification

SVM belongs to a powerful ML tool for both classification and regression [17]. To achieve reasonable classification, the best classification hyper-plane would be searched in training process of SVM. The hyper-plane is determined by an orthogonal weight vector ω that could give the wider margin of separations. Supposing the training dataset is noted as $TD = \left(X_i, Y_i\right), i = 1, 2, ..., l, X \in R^m$, while hyper-plane is $(\omega \cdot X_i + b) = 0$. To ensure all observations can be classified correctly by the hyper-plane, following constraints should be satisfied as:

$$Y_i(\omega \cdot X_i + b) \geq 1, i = 1, 2, ..., l \tag{1}$$

Then the process to maximize the classification margin is defined by:

$$\begin{cases} \min_{\omega,b} \|\omega\|_2^2 / 2 \\ s.t. \quad Y_i(\omega \cdot X_i + b) \geq 1, i = 1, 2, \ldots, l \end{cases} \tag{2}$$

After constructing Lagrange function, this process can be expressed by the Lagrange multiplier α_i as:

$$\begin{cases} \min_{\alpha} \quad \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j \left(X_i \cdot X_j \right) - \sum_{i=1}^{N} \alpha_i \\ \sum_{i=1}^{N} \alpha_i Y_i = 0 \\ \alpha_i \geq 0, \quad i = 1, 2, \ldots, N \end{cases} \tag{3}$$

Based upon equation (3), SVM is capable of not only guaranteeing the accuracy of classification, but also maximizing the blank ranges on all sides of hyper-plane [18].

In order to improve the nonlinear classification performance of SVM, kernel functions should be coupled within SVM. Specifically, through using proper kernel functions, raw data from the original space could be effectively transferred to a high-dimensional space, then the SVM-based classification model could be trained through using the data from this high-dimensional space with the linear classification approach. Supposing $\phi(e)$ is a function to map the input space to a new feature space, the kernel function can be expressed by:

$$K(e, g) = \phi(e) \cdot \phi(g) \tag{4}$$

According to equation (3), the cost function to maximize the classification margin through involving the kernel functions becomes:

$$W(\alpha) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j Y_i Y_j K\left(X_i \cdot X_j \right) - \sum_{i=1}^{N} \alpha_i \tag{5}$$

Based upon the above discussions, kernel functions play the key important roles in determining the classification performance of SVM. It should be known that for different applications, various kernel functions would present different performance, which should be carefully selected. In our study, to well classify the battery electrode property of mass loading, the SVM classification model with four typical and powerful kernel functions are designed and compared.

The first one is the linear kernel with the following form as:

$$K_{linear}(x, z) = a_1 \cdot x^T \cdot z + b_1 \tag{6}$$

Next, two polynomial kernels contain the quadratic kernel and cubic kernel are also utilized in this study as:

$$\begin{cases} K_{quadratic}(x, z) = \left(a_2 \cdot x^T \cdot z + b_2 \right)^2 \\ K_{cubic}(x, z) = \left(a_3 \cdot x^T \cdot z + b_3 \right)^3 \end{cases} \tag{7}$$

The last one is the Gaussian kernel with the following form as:

$$K_{Gaussian}(x,z)=\exp\left[-\frac{\|x-2\|^2}{2\sigma^2}\right] \tag{8}$$

3.2 Performance Indicators

To quantify and investigate the classification performance of proposed SVM with various kernels, some typical performance indicators including the positive predictive value (PPV), false discovery rate (FDR), confusion matrix, true positive rate (TPR), false positive rate (FPR), area under curve (AUC) and receiver operating characteristic (ROC) curve [19] are adopted in this study.

For a multiple classification application, let positive corresponds to an interested class while negative corresponds to other classes, four elements contain true positive (TP), false positive (FP), true negative (TN) and false negative (FN) could be derived for each class. Then for the class C_k (here $k=1:4$), its PPV to quantify the correct rate of class can be calculated by:

$$PPV=\frac{TP}{TP+FP} \tag{9}$$

FDR to quantify the rate of all false discovery of this class can be obtained by:

$$FDR=\frac{FN}{TP+FN} \tag{10}$$

Based upon these two performance indicators, a $(N+1)\times(N+1)$ confusion matrix (CM) to reflect the accuracy of each classification within multi-class problem can be generated. All terms on the primary diagonal of CM represent the correctly-classified results while other terms stand for the incorrect cases of SVM classification.

Next, to further investigate the classification performance of battery multi-class electrode mass loading, the ROC curves of all classes through using different kernel-based SVM is also utilized in this study. It should be known that the ROC curve is generated by plotting TPR against FPR for different threshold settings. Specifically, TPR is used to reflect the number of correct positive classifications happen among all positive observations. FPR provides the amount of incorrect positive classifications happen among all negative observations. The equations of calculating TPR and FPR are expressed as follows:

$$TPR=\frac{TP}{TP+FN} \tag{11}$$

$$FPR=\frac{FP}{FP+TN} \tag{12}$$

After adopting the normalized unit, the AUC of ROC curve can be utilized to reflect the probability that a SVM would rank a randomly-selected positive case higher than a randomly-selected negative case. Better classification approach would generate a classifier point closer to the left-upper corner with a larger AUC value.

4 Result and Discussion

To investigate and quantify the performance of SVMs and the effects of kernel functions on the classification of battery electrode property, the SVM-based framework with various kernels are built and compared for the classification of electrode mass loading in this section.

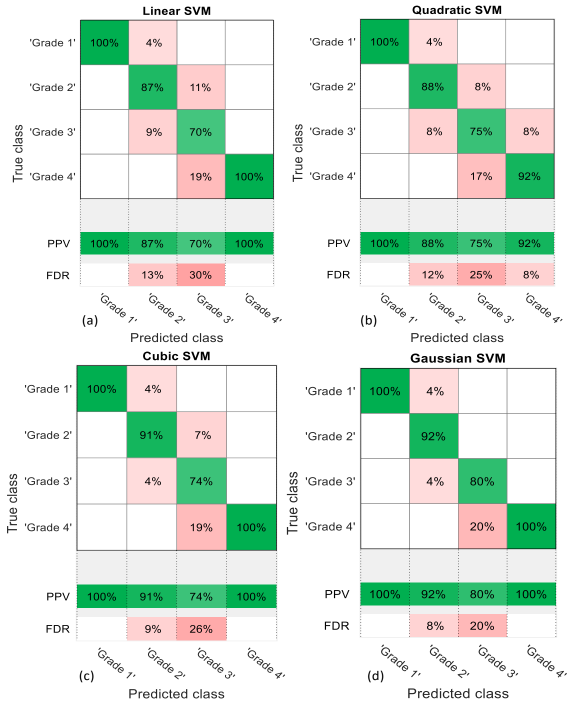

Fig. 2. Confusion matrix for SVM-based classifications with various kernels. a) Linear SVM, b) Quadratic SVM, c) Cubic SVM and d) Gaussian SVM.

Specifically, four product variables consist of the AMMS, STOLR, viscosity and CG are selected as the inputs while the electrode mass loading of battery is utilized as output for all SVM models. After preparing the suitable inputs-output pairs, five folds cross-validation is conducted to train and validate the accuracy and generalization ability of derived SVM models. Fig. 2 illustrates the confusion matrices of all kernel-based SVM classifications. It can be seen that all SVMs present the reliable classification results of all four classes (the PPVs of four SVMs are all larger than 70%), indicating that SVM is capable of effectively classifying the electrode mass loading. Quantitatively, Gaussian kernel-based SVM provides a best classification result with lowest PPV of 80%, indicating the strong nonlinear capture ability of Gaussian kernel. Both cubic kernel-based SVM and quadratic kernel-based SVM present the slight worse classification performance with 74% lowest PPV (7.5% decrease) and 75% lowest PPV (6.3% decrease), respectively. Table 2 illustrates the macro-precision

(*Mac-P*) and micro-F1 score (*Mic-F1*) of all SVM classification results. It can be seen that the *Mac-P* of Gaussian kernel-based SVM reaches 93.0%, which is 1.9%, 4.1% and 4.8% more than that of cubic, quadratic and linear kernel-based SVMs, respectively. The similar trend can be also observed for the *Mic-F1* values of all SVMs. Here the Gaussian kernel-based SVM achieves the best *Mic-F1* with 93.0%, while the *Mic-F1* of linear kernel-based SVM is 86.6% (7.4% decrease). All these facts signify that among these kernel-based SVMs, nonlinear kernel-based SVMs including Gaussian SVM, cubic SVM and quadratic SVM are preferable to achieve better accuracy and generalization ability of battery electrode mass loading classification.

Table 2. Macro precision and micro F1-score of all SVMs with various kernels.

Kernel types	***Mac-P***	***Mic-F1***
Linear kernel	88.8%	86.6%
Quadratic kernel	89.3%	87.8%
Cubic kernel	91.3%	89.1%
Gaussian kernel	93.0%	91.5%

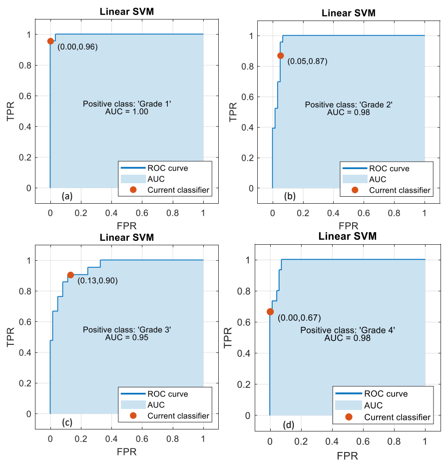

Fig. 3. ROC curves of linear kernel-based SVM classification.

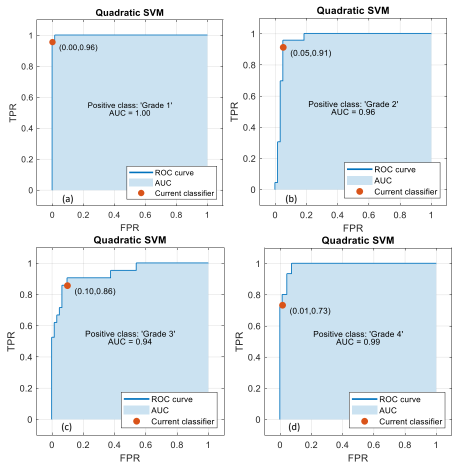

Fig. 4. ROC curves of quadratic kernel-based SVM classification.

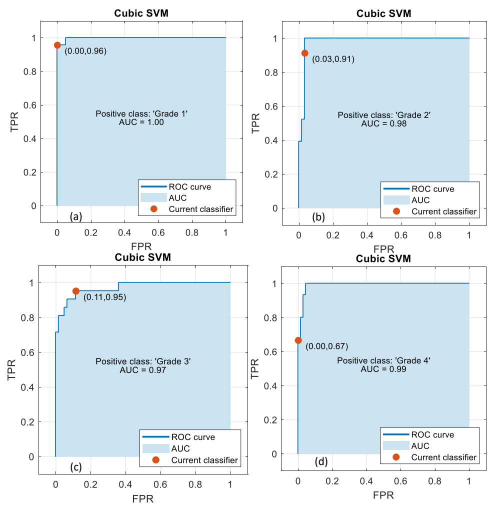

Fig. 5. ROC curves of cubic kernel-based SVM classification.

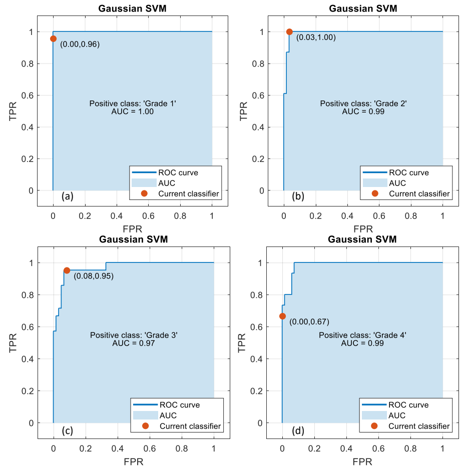

Fig. 6. ROC curves of Gaussian kernel-based SVM classification.

Next, to further investigate the effects of various kernels on each class result, the ROC curves with AUC values and current classifier positions for all four kernel-based SVMs are illustrated in Fig. 3 to Fig. 6, respectively. According to Fig. 3 regarding the linear SVM, grade 1 as the positive class could achieve the best result with 1.00 AUC. Grade 2 and grade 4 achieve the same AUC values of 0.98, indicating the similar classification results for these two class labels. In contrast, grade 3 as the positive class leads to the worst ROC curve with 0.95 AUC. This is mainly caused by several observations from grade 3 are incorrectly classified as the grade 2 (nearly 7%) or grade 4 (nearly 19%) through using linear kernel. For the nonlinear kernel cases, the ROC curves have been effectively improved with larger AUCs. Quantitatively, from Fig. 4 to Fig. 6, the AUCs of grade 4 become 0.99, implying the nonlinear kernels can benefit the classification of grade 4. For the cubic and Gaussian based SVMs, the AUC of grade 3 both become 0.97, which is 2.2% and 3.2% more than that of linear and quadratic cases, respectively. Interestingly, all AUCs of grade 1 are 1.00, which means that grade 1 can be exactly classified through using SVMs. In summary, all kernel-based SVMs can well classify grade 1, while all other grades prefer the nonlinear kernels. Gaussian-based kernel can achieve best classification results for all grades, which is recommended for designing the corresponding SVM framework for electrode mass loading classification.

5 Conclusions

Electrode property plays an important role in determining the final battery performance, which should be carefully classified and analyzed. In this study, an effective data-driven classification method, based on the SVM with various kernels, is proposed to well classify the battery electrode mass loading and analyze the effects of four product features (AMMC, STOLR, viscosity, CG) from mixing and coating steps. The classification performance of linear, quadratic, cubic and Gaussian kernel-based SVMs are all systematically investigated and compared through using different performance indicators and ROC curves. Illustrative results demonstrate that Gaussian kernel based SVM is capable of achieving the best classification results among four kernels (here is 93.0% *Mac-P* and 91.5% *Mic-F1).* Besides, the labelled grade 1 of electrode mass loading can be exactly classified by SVM with all kernels. The labelled grade 3 presents the worst classification results (here the worst AUC is 0.94) of all kernel cases, which should be reset to further improve the classification performance. This proposed kernel-based SVM framework actually belongs to a data-driven approach, which can be conveniently extended to classify other product properties and analyze other variables in battery production domain.

References

1. K. Liu, K. Li, Q. Peng, and C. Zhang. A brief review on key technologies in the battery management system of electric vehicles. Frontiers of Mechanical Engineering 14, no. 1, 47-64, (2019).
2. A. Kwade, W. Haselrieder, R. Leithoff, A. Modlinger, F. Dietrich, and K. Droeder. Current status and challenges for automotive battery production technologies. Nature Energy 3, no. 4 (2018): 290-300.
3. Y. Li, K. Liu, A. M. Foley, A. Zülke, M. Berecibar, E. N. Maury, J. V. Mierlo, and H. E. Hoster. Data-driven health estimation and lifetime prediction of lithium-ion batteries: A review. Renewable and Sustainable Energy Reviews 113, 109254 (2019).
4. Y. Guo, Z. Yang, K. Liu, Y. Zhang, and W. Feng. A compact and optimized neural network approach for battery state-of-charge estimation of energy storage system. Energy 219 (2021): 119529.
5. X. Hu, F. Feng, K. Liu, L. Zhang, J. Xie, and B. Liu. State estimation for advanced battery management: Key challenges and future trends. Renewable and Sustainable Energy Reviews 114, 109334, (2019).
6. K. Liu, Y. Li, X. Hu, M. Lucu, and W. D. Widanage, Gaussian process regression with automatic relevance determination kernel for calendar aging prediction of lithium-ion batteries. IEEE Transactions on Industrial Informatics 16, no. 6 3767-3777 (2019).
7. X. Tang, K. Liu, X. Wang, F. Gao, J. Macro, and W. D. Widanage. Model migration neural network for predicting battery aging trajectories. IEEE Transactions on Transportation Electrification (2020).
8. K. Liu, K. Li, and C. Zhang. Constrained generalized predictive control of battery charging process based on a coupled thermoelectric model. Journal of Power Sources 347, 145-158 (2017).
9. Q. Ouyang, Z. Wang, K. Liu, G. Xu, and Y. Li. Optimal Charging Control for Lithium-Ion Battery Packs: A Distributed Average Tracking Approach. IEEE Transactions on Industrial Informatics 16, no. 5 (2019): 3430-3438.
10. Y. Shang, K. Liu, N. Cui, N. Wang, K. Li, and C. Zhang. A Compact Resonant Switched-Capacitor Heater for Lithium-Ion Battery Self-Heating at Low Temperatures. IEEE Transactions on Power Electronics 35, no. 7 (2019): 7134-7144.

11. J. Wu, Z. Wei, K. Liu, Z. Quan, and Y. Li. Battery-involved Energy Management for Hybrid Electric Bus Based on Expert-assistance Deep Deterministic Policy Gradient Algorithm. IEEE Transactions on Vehicular Technology 69, no. 11 (2020): 12786-12796.
12. K. Liu, Z. Wei, Z. Yang, K. Li, Mass load prediction for lithium-ion battery electrode clean production: a machine learning approach. Journal of Cleaner Production 289 (2021): 125159.
13. J. Schnell, G. Reinhart, Quality management for battery production: a quality gate concept. Procedia CIRP, 57, pp.568-573 (2016).
14. J. Schnell, C. Nentwich, F. Endres, A. Kollenda, F. Distel, T. Knoche, and G. Reinhart, Data mining in lithium-ion battery cell production. Journal of Power Sources 413, 360-366, (2019).
15. A. Turetskyy, S. Thiede, M. Thomitzek, N. V. Drachenfels, T. Pape, and C. Herrmann, Toward Data-Driven Applications in Lithium-Ion Battery Cell Manufacturing. Energy Technology, 1900136, (2019).
16. R. P. Cunha, T. Lombardo, E. N. Primo, and A. A. Franco, Artificial Intelligence Investigation of NMC Cathode Manufacturing Parameters Interdependencies. Batteries & Supercaps 3, no. 1, 60-67, (2020).
17. W. S. Noble, What is a support vector machine?. Nature biotechnology 24, no. 12 (2006): 1565-1567.
18. P. Rebentrost, M. Mohseni, and S. Lloyd. Quantum support vector machine for big data classification. Physical review letters 113, no. 13 (2014): 130503.
19. K. Liu, X. Hu, H. Zhou, L. Tong, D. Widanalage, and J. Macro. Feature analyses and modelling of lithium-ion batteries manufacturing based on random forest classification. IEEE/ASME Transactions on Mechatronics (2021).