Journal of Quantum Computing
DOI:10.32604/jqc.2021.016390
Article

Tech Science Press

Lifetime Prediction of $LiFePO_4$ Batteries Using Multilayer Classical-Quantum Hybrid Classifier

Muhammad Haris[1,*], Muhammad Noman Hasan[1], Abdul Basit[2] and Shiyin Qin[1]

[1]School of Automation Science and Electrical Engineering, Beihang University, Beijing, 100083, China
[2]China Academy of Space Technology, Shenzhou Institute, Beijing, 100010, China
[*]Corresponding Author: Muhammad Haris. Email: haris.capricorn@gmail.com
Received: 02 May 2021; Accepted: 10 August 2021

Abstract: This article presents a multilayer hybrid classical-quantum classifier for predicting the lifetime of $LiFePO_4$ batteries using early degradation data. The multilayer approach uses multiple variational quantum circuits in cascade, which allows more parameters to be used as weights in a single run hence increasing accuracy and provides faster cost function convergence for the optimizer. The proposed classifier predicts with an accuracy of 92.8% using data of the first four cycles. The effectiveness of the hybrid classifier is also presented by validating the performance using untrained data with an accuracy of 84%. We also demonstrate that the proposed classifier outperforms traditional machine learning algorithms in classification accuracy. In this paper, we show the application of quantum machine learning in solving a practical problem. This study will help researchers to apply quantum machine learning algorithms to more complex real-world applications, and reducing the gap between quantum and classical computing.

Keywords: Classical-quantum; classifier; quantum machine learning; classification; $LiFePO_4$; Lithium-ion

1 Introduction

Quantum computers promise to solve the complex problems of the world, which would be impossible for classical computing machines by offering groundbreaking exponentially faster computation. However, the fully developed fault-tolerant quantum computers will still take some years to come. The concept of hybrid classical-quantum computing algorithm development is becoming popular for the first generation of the quantum computer. The combination of machine learning with the quantum computing reveals surprising results. The advantage to process quantum coherence and entanglement gives quantum computing a sharp edge over classical computations. Quantum computing provides square-root speedup as compared to traditional machine learning techniques [1]. The proposed classifier is based on a multilayer variational circuit which provides better accuracy. The variational circuit opens a new era of research in the field of quantum learning. Some of the variational circuit-based quantum classifiers are presented in [2–4]. We also show the importance of combining classical computing with quantum computing in the actual classification task through this paper. The results of the study will help in early prognostics of lithium-ion batteries.

Lithium-ion has high energy density, long maintenance-free life, and low carbon emission profile. These characteristics make lithium-based batteries suitable candidates for usage in laptops, cell-phones, power tools, and electric vehicles (EV) as energy storage devices [5–6]. Lithium-ion has high energy efficiency, which also improves the power quality of renewable energy systems like wind and solar energy. Therefore, industry and, government agencies are giving more importance to lithium-based energy storage systems. Lithium iron phosphate ($LiFePO_4$) is one of the important lithium-based batteries with high specific experimental capacity (165 mAh g^{-1}) [7–8]. Lithium-ion suffers degradation during its lifetime.

During initial cycles, this degradation is caused by the initial formation of SEI and depletion of mobile lithium of anode. The main reason of capacity degradation is due to the decrease in lithium inventory (LLI) and loss of active cathode including, lithiated material loss and particle cracking [9–11]. This chemical degradation is influenced by operating temperature, charge and discharge rate, operating depth of discharge (DOD), and charging protocol [12–14].

Model and data-driven based lithium-ion remaining useful lifetime predictions is a relatively new area of research. Researchers are using statistical and machine learning algorithms for estimating the remaining useful lifetime and in prognostics and health management of lithium-ion batteries [15–16]. These algorithms include statistical models such as Kalman filter [17], Gaussian process regression [18–19], Dempster Shafer theory and Bayesian Monte Carlo method [20], k-nearest neighbors [21] and artificial intelligence techniques like deep learning methods [22–25].

Life cycle predictions of lithium-ion batteries in the early stages of the operation will help in the faster development of large battery banks. In this study, we develop a data-driven hybrid classical-quantum prediction model using initial degradation data of the $LiFePO_4$ in fast charging application. This study uses data of the initial four cycles to classify the life cycle of the lithium-ion battery into long and short lifetime groups. It will help manufacturers to predict the life of the battery in initial stages without going through the long cycling durations saving the development time. We demonstrate that our classifier will classify with an accuracy of greater than 92.8% despite computational complexity. In this study, we use the degradation data published in [26]. This dataset is generated by applying multistep fast charging on $LiFePO_4$ cells. The fast charging of lithium-ion cells is of great interest to the consumer electronics industry nowadays.

The contribution of this paper is to present multilayer hybrid classical-quantum classifier and use it to predict the remaining lifecycle of the lithium-ion batteries. The article is organized as follows. Section 2 provides details of proposed classical-quantum classifier. Section 3 discuss the testing procedures and data generated from [26]. Section 4 present the experimental results of the model and performance evaluation. The conclusion is drawn in Section 5.

2 Multilayer Classical-Quantum Classifier

2.1 Basic Principle

The primary concept is based on variational Eigen-solver, which was proposed to find the lowest energy state of a quantum system. The main purpose behind the proposed classifier is to develop a quantum device to calculate the value of an objective function f (θ) for a given set of classical parameters θ. A classical algorithm will minimize the outcome f (θ) by optimizing the parameter θ by reiteratively running the quantum device.

Let us assume a Hamiltonian $\mathcal{H}$ of quantum system S having N qubits. The Hamiltonian $\mathcal{H}$ having eigenvectors η_i and eigenvalues λ_i. Such that, $\lambda_1 \leq \lambda_2 \leq \lambda_3 \ldots \leq \lambda_N$ and λ_1 correspond to the lowest energy state of the system. The expectation value of the Hamiltonian with respect to state $|\psi\rangle$ is given by Eq. (1).

$$\langle \mathcal{H} \rangle_{|\Psi\rangle} = \frac{\langle \Psi|\mathcal{H}|\Psi\rangle}{\langle \Psi|\Psi\rangle} \tag{1}$$

Consider a vector $\vec{\theta}$ having real-valued parameters $\theta_j$and we apply this vector to the Hamiltonian of the system S. If we prepare quantum state variable depending upon the vector θ_j, such that $|\Psi(\vec{\theta})\rangle$. The variational method of quantum mechanics states that:

$$\langle \mathcal{H} \rangle_{|\Psi(\vec{\theta})\rangle} \equiv \langle \mathcal{H} \rangle(\vec{\theta}) = \langle \Psi(\vec{\theta})|\mathcal{H}|\Psi(\vec{\theta})\rangle \geq \lambda_1 \tag{2}$$

The main objective is to optimize the selection of $\vec{\theta}$, which minimizes $\langle \mathcal{H} \rangle(\vec{\theta})$ as shown in Fig. 1.

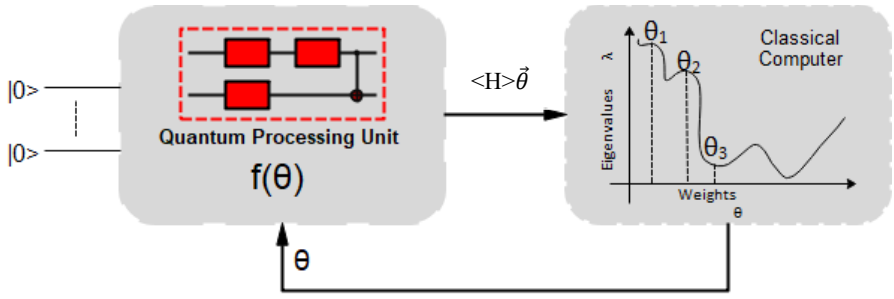


Figure 1: A classical-quantum method to find the lowest energy state of the system

2.2 Quantum Encoding

The dataset for training and validation should be represented into quantum states in order to process it by a quantum computer called state preparation or quantum encoding. Amplitude encoding is adopted to encode our dataset into quantum states in order to process by our quantum circuit. The most significant advantage of amplitude encoding is that only log(XY) qubits are required to represent the data of Y features and X inputs as compared to processing required by classical machine with some linear function of XY [27].

The states of our dataset are prepared by the method proposed in [28] using multi-controlled rotation of qubits. In this method, we perform different uniformly controlled rotations for each branch of superposition based on the amplitude of the input vector. The controlled rotation with angle β in quantum circuits is a gate $G_m^l(\vartheta_{x,y,z},\beta)$ of one controlled qubit on m target qubits in x, y or z-axis. Consider an input vector $(\vec{x})$, the state preparation is done by applying controlled rotation $G_m^{m-1}(\vartheta_y,\beta)$ on the y-axis. It will zero all the vectors corresponding to the states equivalent to bit value one in the qubit m.

$$G_m^{m-1}(\vartheta_y,\beta)|\hat{x}\rangle = \left(x_{1,2},0,x_{2,2},0,\dots,a_{\frac{N}{2},2},0\right)^T \tag{3}$$

This method is repeated for all non-zero elements.

$$G_m^{m-1}(\vartheta_y,\beta)|\hat{x}\rangle = \left(x_{1,2},x_{2,2},\dots,a_{\frac{N}{2},2}\right)^T \oplus (1,0)^T \tag{4}$$

On gate level, it can be achieved using CNOT gate and one qubit rotation on the y-axis for m-1 controlled qubits. Fig. 2 shows the state preparation circuit for two qubits on y rotation. The angles for rotation β related to the amplitude of input vector $\vec{x}$, can be found by Eq. (5).

$$\beta_j^m = 2sin^{-1}\left(\frac{\sqrt{\sum_{o=1}^{2^{m-1}}\left|x_{(2j-1)2^{s-1}+o}\right|^2}}{\sqrt{\sum_{o=1}^{2^m}\left|x_{(j-1)2^s+o}\right|^2}}\right) \tag{5}$$

Here, $j = 1,2,\dots,2^{l-m}$.

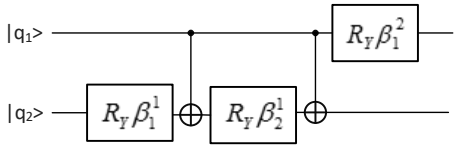


Figure 2: Quantum circuit for state preparation

2.3 Multilayer Quantum Circuit for Classification

Our basic quantum circuit is a two-qubit circuit having unitary operations depends upon the rotation angle (θ), U (θ). For this purpose, we design a simple quantum circuit that provides single-qubit rotation to both qubits and entangles them by CNOT gate, which makes up a single quantum circuit layer. This basic layer is used in series to make a multilayer quantum circuit. In the final stage, measurements of the states are

calculated through Pauli operators. Like classical machine learning, the rotation angle θ is adjusted by a back-propagation algorithm on the classical computer after measuring the cost function of the quantum circuit.

The biggest advantage of using this multilayer technique is that the classical computer can adjust a larger set of rotation angles in a single epoch. It provides faster con-vergence for optimizer and gives higher accuracy. The quantum circuit first produces initial cost function C (θ) using initial parameters which are given by Eq. (6).

$$C(\theta) = \langle \Psi(\vec{\theta}) | \mathcal{H} | \Psi(\vec{\theta}) \rangle \quad (6)$$

The classical computing algorithm then reiteratively lowers the energy by evaluating cost function and minimizing it using optimizers. Fig. 3 shows the complete block diagram of the multilayer classical-quantum hybrid classifier. The rotation angles in the quantum circuit are initialized to a random value. The rotation angles (weights) are updated in every iteration to minimize the cost function.

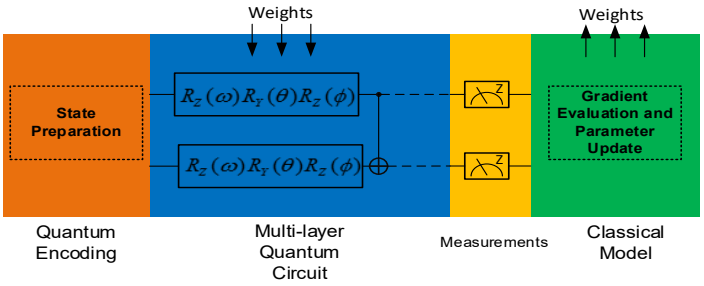
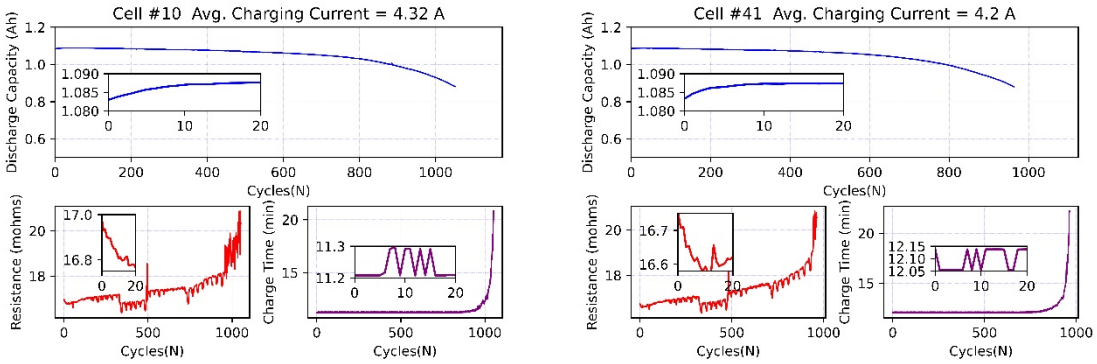


Figure 3: Multilayer classical-quantum classifier

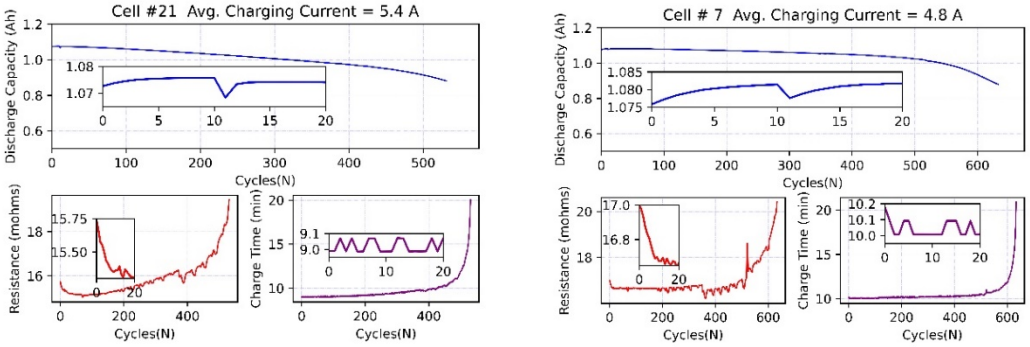
3 Experimental Data

For our analysis and classification, we use lithium-ion capacity degradation data from [26]. The aging is performed by charging in CC-CV charging protocol at different multistep fast charging rates on 124 commercially available cells. The test was per-formed in three batches at different time. Among them, we have selected data from one batch, which consists of degradation data of 46 cells for training and validation. The data is divided randomly into training and testing data, having 30% data for validation of the model. The failure criteria are set to be 20% decrease in the initial capacity of the cells. Fig. 4 shows a glimpse of different features present in the data, correlate to the aging of four cells selected randomly at different charging protocols.

Unlike [26], we use data of only the first four cycles for our analysis and divided our results into two groups, long lifecycle (>= 700 cycles) and short lifecycle (<700 cycles) based on the 80% remaining discharge capacity threshold. As shown in Fig. 4, the data does not show any sign of degradation in the capacity of the batteries at initial stage. We extract four features for the classifier from average charging current, impedance, charging time, and discharging profile.



(a) (b)



(c) (d)

Figure 4: Degradation curves of the four randomly selected cells from the dataset charged at different rates. The inset graph shows the detail view of the initial 20 cycles. (a) Degradation at 4.32A charging current. (b) Degradation at 4.2A charging current. (c) Degradation at 5.4A (40%) and 3.6 (60%) charging current (d) Degradation at 4.8A charging current

4 Results and Discussion

The quantum circuit was run on a prototype quantum processor to verify the functionality through the actual quantum device through IBM Q Experience [29]. The quantum circuit consists of 5 layers to use as a classifier. The hybrid model was tested through three different back-propagation optimizer: Adam [30], AdaGrad [31], and Nesterov accelerated gradient [32]. Nesterov accelerated gradient showed the best convergence capability and, we use it to minimize the cost function. Table 1 enlists the parameters for the Multilayer Quantum Circuit (MQC) and Classical Computing Unit (CCU) of the classifier. The classifier gives 12.5% and 7.2% of misclassification error on training and testing datasets, respectively. We also test our classifier with another batch of 44 lithium-ion data to verify the universality of the classifier. The misclassification error for the new and untrained data is only 16%, which shows that the classifier can be used to predict the lifecycle of the same model very uniquely. Table 2 shows the classification accuracy of the classifier on testing data and untrained data.

Table 1: Characteristics and parameters of the multilayer quantum circuit and classical computing unit

Multilayer Quantum Circuit	**Qubits**	**2**
	Layers	**5**
	Quantum encoding	**Amplitude Encoding**
	Number of gates for each layer	**7**
Classical Computing Unit	Batch Size	4
	Optimizer	Nesterov Accelerated Gradient
	Optimizer step size	0.01
	Loss function	Squared Loss

Table 2: Model metrics of the classifier on trained and untrained data

	Training accuracy (%)	**Validation accuracy (%)**
Trained data	87.5	92.8
Untrained data		84

The benchmarking is performed by comparing the proposed classifier with classical binary classifiers. Fig. 5 shows the comparison among different classifiers based on Area Under the Receiving Operating Curve (AUROC) criteria. The proposed multilayer hybrid classical-quantum classifier shows better performance than other classifiers.

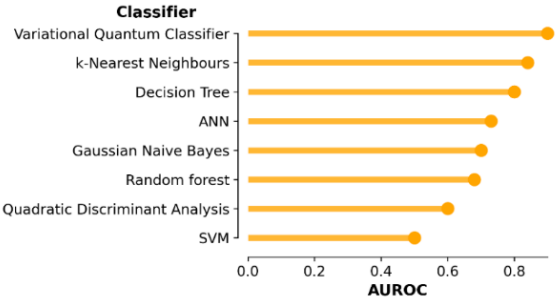


Figure 5: Performance comparison between proposed classifier and classical binary classifiers on same dataset

5 Conclusion

In this article, we present a multilayer hybrid classical-quantum classifier and display its application in prognostics application and compare it with classical algorithms. The proposed classifier and its application for prognostics is novel. The model is trained from data of the initial four cycles, and we obtain only 7.2% error in the testing data. The model gives excellent results (84% accuracy) when predicting lifetime groups using untrained data. Our future work will focus on developing a full-scale quantum model for estimating cost function as well in prognostics application and increasing the accuracy of the classifier.

Acknowledgement: We are grateful to the peoples for the support and encouragement.

Funding Statement: The authors received no specific funding for this study.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

References

[1] J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost, N. Wiebe *et al.,* "Quantum machine learning," *Nature*, vol. 549, no. 7671, pp. 195–202, 2017.

[2] M. Schuld, A. Bocharov, K. Svore and N. Wiebe, "Circuit-centric quantum classifiers," *Physical Review A*, vol. 101, no. 3, pp. 32308–32325, 2020.

[3] K. Mitarai, M. Negoro, M. Kitagawa and K. Fujii, "Quantum circuit learning," *Physical Review A*, vol. 98, no. 3, pp. 32309–32315, 2018.

[4] E. M. Gil Fuster, "Variational quantum classifier," *Physical Review A*, vol. 96, no. 1, pp. 31208–31216, 2017.

[5] Y. Miao, P. Hynan, A. von Jouanne and A. Yokochi, "Current Li-ion battery technologies in electric vehicles and opportunities for advancements," *Energies*, vol. 12, no. 6, pp. 1–20, 2019.

[6] T. Kim, W. Song, D. Y. Son, L. K. Ono and Y. Qi, "Lithium-ion batteries: Outlook on present, future, and hybridized technologies," *Journal of Materials Chemistry A*, vol. 7, no. 7, pp. 2942–2964, 2019.

[7] N. Nitta, F. Wu, J. T. Lee and G. Yushin, "Li-ion battery materials: Present and future," *Materials Today*, vol. 18, no. 5, pp. 252–264, 2015.

[8] R. Ruffo, R. A. Huggins, C. M. Mari, M. Piana and W. Weppner, "Phosphate materials for cathodes in lithium ion secondary batteries," *Ionics*, vol. 11, no. 3–4, pp. 213–219, 2005.

[9] A. Jz, B. Msdda, B. Mka, C. Drs and C. Mha, "Investigation of lithium-ion battery degradation mechanisms by combining differential voltage analysis and alternating current impedance," *Journal of Power Sources*, vol. 448, no. 1, pp. 28–30, 2020.

[10] K. Uddin, S. Perera, W. D. Widanage, L. Somerville and J. Marco, "Characterising lithium-ion battery degradation through the identification and tracking of electrochemical battery model parameters," *Batteries*, vol. 2, no. 2, pp. 1–10, 2016

[11] L. de Biasi, B. Schwarz, T. Brezesinski, P. Hartmann and J. Janek, "Chemical, structural, and electronic aspects of formation and degradation behavior on different length scales of Ni-rich NCM and Li-rich HE-NCM cathode materials in Li-ion batteries," *Advanced Materials*, vol. 31, no. 26, pp. 1900985–1900995, 2019.

[12] C. Zhang, F. Yan, C. Du, J. Kang and R. F. Turkson, "Evaluating the degradation mechanism and state of health of $LiFePO_4$ lithium-ion batteries in real-world plug-in hybrid electric vehicles application for different ageing paths," *Energies*, vol. 10, no. 1, pp. 1–10, 2017.

[13] C. Liu, J. Tan, H. Shi and X. Wang, "Lithium-ion cell screening with convolutional neural networks based on two-step time-series clustering and hybrid resampling for imbalanced data," *IEEE Access*, vol. 6, no. 1, pp. 59001–59014, 2018.

[14] Y. Zhang, J. Xu, S. Yang, C. Deng, F. Chen *et al.,* "Battery module capacity fade model based on cell voltage inconsistency and probability distribution," *Advances in Mechanical Engineering*, vol. 9, no. 9, pp. 168781401773075–168781401773085, 2017.

[15] D. N. T. How, M. A. Hannan, M. S. Hossain Lipu and P. J. Ker, "State of charge estimation for lithium-ion batteries using model-based and data-driven methods: A review," *IEEE Access*, vol. 7, no. 1, pp. 136116–136136, 2019.

[16] H. Meng and Y. F. Li, "A review on prognostics and health management (PHM) methods of lithium-ion batteries," *Renewable and Sustainable Energy Reviews*, vol. 116, no. 1, pp. 1–11, 2019.

[17] Z. Yu, R. Huai and L. Xiao, "State-of-charge estimation for lithium-ion batteries using a Kalman filter based on local linearization," *Energies*, vol. 8, no. 8, pp. 7854–7873, 2015.

[18] P. Tagade, "Deep Gaussian process regression for lithium-ion battery health prognosis and degradation mode diagnosis," *Journal of Power Sources*, vol. 445, no. 1, pp. 227281–227291, 2020.

[19] D. Yang, X. Zhang, R. Pan, Y. Wang and Z. Chen, "A novel Gaussian process regression model for state-of-health estimation of lithium-ion battery using charging curve," *Journal of Power Sources*, vol. 384, no. 1, pp. 387–395, 2018.

[20] W. He, N. Williard, M. Osterman and M. Pecht, "Prognostics of lithium-ion batteries based on Dempster-Shafer theory and the Bayesian Monte Carlo method," *Journal of Power Sources*, vol. 196, no. 23, pp. 10314–10321, 2011.

[21] Y. Zhou, M. Huang and M. Pecht, "Remaining useful life estimation of lithium-ion cells based on k-nearest neighbor regression with differential evolution optimization," *Journal of Cleaner Production*, vol. 249, no. 1, pp. 1–11, 2020.

[22] P. Khumprom and N. Yodo, "A data-driven predictive prognostic model for lithium-ion batteries based on a deep learning algorithm," *Energies*, vol. 12, no. 4, pp. 1–21, 2019.

[23] S. Shen, M. Sadoughi, X. Chen, M. Hong and C. Hu, "A deep learning method for online capacity estimation of lithium-ion batteries," *Journal of Energy Storage*, vol. 25, no. 1, pp. 100817–100827, 2019.

[24] G. Zhao, G. Zhang, Y. Liu, B. Zhang and C. Hu, "Lithium-ion battery remaining useful life prediction with Deep Belief Network and Relevance Vector Machine," in *IEEE Int. Conf. on Prognostics and Health Management*, pp. 7–13, 2017.

[25] S. Shen, M. Sadoughi and C. Hu, "Online estimation of lithium-ion battery capacity using transfer learning," in *IEEE Transportation Electrification Conf. and Expo*, pp. 1–4, 2019.

[26] K. A. Severson, P. M. Attia, N. Jin, N. Perkins and B. Jiang, "Data-driven prediction of battery cycle life before capacity degradation," *Nature Energy*, vol. 4, no. 5, pp. 383–391, 2019.

[27] M. Schuld and F. Petruccione, "Information encoding," in *Supervised Learning with Quantum Computers*. Springer, Cham, 2018, pp. 139–171.

[28] M. Möttönen, J. J. Vartiainen, V. Bergholm and M. M. Salomaa, "Transformation of quantum states using uniformly controlled rotations," *Quantum Physics*, vol. 5, no. 467, pp. 1–12, 2005.

[29] "IBM Quantum Experience-Dashboard" [Online]. Available: https://quantum-computing.ibm.com/.

[30] D. P. Kingma and J. L. Ba, "Adam: A method for stochastic optimization," in *3rd Int. Conf. for Learning Representations,* San Diego, pp. 1–15, 2015.

[31] J. Duchi, E. Hazan and Y. Singer, "Adaptive subgradient methods for online learning and stochastic optimization," in *23rd Annual Conf. on Learning Theory*, pp. 257–269, 2010.

[32] A. Botev, G. Lever and D. Barber, "Nesterov's accelerated gradient and momentum as approximations to regularised update descent," in *Proc. Int. Joint Conf. on Neural Networks*, vol. 2017, no. 2, pp. 1899–1903, 2017.