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A Physically Inspired Equivalent Neural Network Circuit Model for SoC Estimation of Electrochemical Cells

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Abstract: Battery Management System (BMS) design for Lithium-ion batteries State of Charge (SoC) prediction has a crucial role in Electric Vehicles (EVs) and smart grids development. The need to design compact, light and fast devices requires finding a suitable trade-off between effectiveness and efficiency. In the literature, it is well emphasized that the application of electrochemical-based methods such as the Pseudo-Two-Dimensional (P2D) model is computationally prohibitive and requires significant simplifications. Conversely, plain Equivalent Circuit Models (ECM) are too simple and unable to represent the cell dynamics. The application of an Ensemble Neural Network (ENN) as Equivalent Neural Network Circuit (ENNC) emerged as a promising solution able to synthesize expressive and computationally efficient models. Indeed, with the support of a suitable dataset, an ENN can be configured to represent a given ECM, modeling each lumped parameter through an assigned Neural Network (NN). Accordingly, the ENNC system is able to keep a physical description of the battery cell while approximating the non-linear dynamic of each component. The paper proposes a novel ENNC battery named Physical Inspired-Equivalent Neural Network Circuit (PI-ENNC) whose ensemble architecture relies on a fractional-order Extended Single Particle (ESP) Lithium-ion cell formulation. The PI-ENNC is designed to approximate the ESP transfer functions referred to the ohmic effects, the electrolyte diffusion and the non-uniform charge distribution in the cell. The proposed model has been tested with three publicly available datasets, investigating the model behavior according to two different training strategies and with different input configurations. In order to prove its effectiveness, results have been compared with a simpler version proposed in a previous work. Results highlight the effectiveness of PI-ENNC in SoC prediction, underlining the importance of designing an ENN architecture that leverages on equations and constraints that reflect the physical phenomena of the cell.

Keywords: battery management system; neural networks; Li-ion battery; ensemble neural network; circuit equivalent models; state of charge; prediction; machine learning; data driven

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1. Introduction

Li-Ion batteries emerge as the main Energy Storage System (ESS) technology in the automotive field and smart grids for the integration of renewable energy sources, electric mobility, Vehicle to Grid (V2G) systems and demand response programs into the electric grid [1–4]. With respect to other technologies, Lithium-Ion batteries are characterized by high energy densities, fast-response and competitive costs. In [2,5], the authors reported a detailed review on the Lithium-Ion ESS applications in automotive and V2G systems, highlighting the increasing efforts in the research field as well as all the progress in energy management, safety issues and cost abatement. Concerning the latter, Lithium-Ion batteries costs have been reduced by 70% in the last decade. Although the price is still considerably high ("500 ($/kWh) that is about USD 35,000 to 40,000 of the overall EVs' price" [2]), it is expected to reach values lower than 200 ($/kWh) [6].

In addition to possible improvements in chemical materials, cell design and circuital components, the research activity directions move towards the optimization of intelligent Battery Management System (BMS) devices to improve the reliability of the battery pack. The BMS is in charge of monitoring and managing every cell inside the battery system ensuring that their working points are bounded within the safety area [7]. Moreover, the excessive charging/discharging currents and power transients should be monitored by the BMS avoiding possible damages and deterioration of the battery cell. Usually, its working frequency is equal or greater than one second and its hardware must be as light and compact as possible in order to fit into an Electric Vehicle (EV) [8]. A detailed study on the hardware design, functioning and BMS architecture is discussed in [7,9].

Designing an effective and efficient prediction model able to approximate the cell dynamic and thus its State of Charge (SoC) is a crucial facet for BMS systems, as widely emphasized in the literature [10–12]. Indeed, other than maximizing the prediction effectiveness, the BMS algorithm should be characterized by low computational costs.

Amongst the prediction models proposed in the literature, *direct methods* emerged as the most popular approaches due to their intuitive reasoning and ease of implementation. Indeed, they are only based on "Direct measures of physical battery properties such as voltage, current, and temperature, and then, by using an equation or relationship" [13]. Typical examples of direct methods are Coulomb Counting (CC) estimation [14], the Open Circuit Voltage (OCV) estimation and the Electrochemical Impedance Spectroscopy (EIS) estimation [13,15,16]. By leveraging on a limited number of equations, relations and direct measures, these methods appear very efficient in terms of computational cost and ease of implementation.

However, SoC estimation techniques based on direct measures, i.e., OCV methods and CC algorithms, are not satisfactory for the battery pack installation in complex power systems like automotive systems and smart grids which usually show high power peaks and power transients. Indeed, these models are not able to take into account the ohmic and the electrolyte diffusion effects in the cell, which produce very high uncertainties during power transients. This phenomenon is well described in [17] by means of a mechanical analogy. In the manuscript, the problem of estimating the amount of charge stored in a cell based on voltage and current measurements has been associated with the problem of estimating the volume of the water stored in a reservoir based on pressure and flow rate measurements.

Even though CC is widely adopted [3,18,19], in [20,21], the authors described four types of error sources that can compromise the accuracy of the SoC prediction. These can be summarized in: (i) current measurement error; (ii) error due to the approximation of current integration with respect to time; (iii) uncertainty in the knowledge of battery capacity; and the (iv) error (drift) in timing oscillator.

Considering the same approach, three types of error are summarized also for voltage-based (or OCV-based) models [21]: (i) OCV-SOC modeling error; (ii) voltage-drop modeling error; (iii) voltage measurement error.

For the motivations discussed above, the authors suggest the implementation of suitable filters supporting the prediction model to improve the SoC estimation. Non-linear Kalman Filters (KFs) such as Extended Kalman Filter (EKF) [22] and Unscented Kalman Filter (UKF) [23] emerge as interesting and widely adopted solutions for this purpose as well as Recursive Least Square, Particle and H-infinity filters [11,13].

In order to design more effective BMSs, non-linear KFs are usually supported with accurate prediction models impacting on the computational costs of the procedure as discussed in [24–28].

In the literature, there are several surveys and reviews concerning the categorization of BMS prediction models. In [9], the authors distinguished three main approaches: electrochemical models, Equivalent Circuit Models (ECMs) and black box models. A similar categorization is proposed in [11,29], where authors summarize the SoC estimation methods into direct measures, computational intelligence and model-based approaches [11],

whereas in [29], they are distinguished by electrochemical, empirical-ECM and empirical-Neural Networks (NNs).

Electrochemical models are based on high-order differential equations representing the chemical and electrochemical kinetics, as well as the mechanical and transport laws used to simulate the Li-ion battery's characteristics and reactions. These models can accurately predict physical quantities through a fine tuning of the model coefficients and parameters. However, they are usually characterized by considerably high computational costs. Indeed, electrochemical models consist in high order differential equations, such as Pseudo-two-Dimensional (P2D) models [30], which are not suitable for online applications. For this reason, P2D models are often reformulated in order to provide a good trade-off between the prediction accuracy and computational costs [31–35].

Conversely, ECMs are featured by fewer (lumped) parameters and they are often used in online applications. Indeed, these models are linear (or piece-wise linear) systems that can be represented by an equivalent electric circuit. However, in most cases they lack physical interpretation and can only provide the description of high-level physical quantities [12]. In many studies, ECMs models have been tuned offline according to a suitable optimization algorithm since the real lumped parameter values are hardly ever known a priori. Evolutionary algorithms and Swarm Optimization approaches such as Particle Swarm Optimization (PSO) have been proved to be effective solutions for correctly determining meaningful values for the ECM parameters [36–40].

Regarding black box models, they describe a linear or non-linear mapping function of battery voltage response characteristics [9]. According to [11,29], these models rely on machine learning algorithms and data driven techniques. Therefore, they neglect the internal mechanisms of the cell and do not provide further physical explanation of the cell behavior since the model is learned by considering only the dataset at hand. Concerning the models proposed in the literature, Fuzzy Inference Systems (FISs) [41,42], NNs [43–47] and Support Vector Machines (SVMs) [48,49] have been widely explored.

Beyond the categorizations written above, it is interesting to highlight the following points. In the case of an electrochemical model, a suitable simplification and problem linearization can collapse its transfer functions into an ECM representation, that is, when the differential equations are simplified (i.e., truncated) to the first-order as in [16,34]. An ECM can be synthesized through a suitable machine learning model, (e.g., NNs, SVMs or FISs) in order to tune the lumped parameters non-linearities according to the available dataset representing the cell for approximation. This approach would be able to provide some degree of interpretability of the ECM moving toward a white box equivalent model [9,46].

As proposed in [46], the application of Equivalent Neural Network Circuits (ENNCs) based on Ensemble Neural Network (ENN) systems [50] is an interesting solution. Indeed, a given ENN can be configured to reproduce a corresponding ECM by assigning each NN of the ensemble system to an ECM lumped parameter in order to better approximate the circuit non-linearities and therefore the cell behavior. In this paper, a Physical Inspired Equivalent Neural Network Circuit (PI-ENNC) is proposed as an extension of the ENNC introduced in [46]. The ENN architecture of PI-ENNC has been conceived to attain a strong analogy with the ESP fractional-order model proposed in [34]. The tests are focused on an exhaustive comparison between the ENNC and the PI-ENNC considering the SoC prediction and different training procedure and dataset.

The main contributions of this work can be summarized as follows:

- An exhaustive description of the ENNC model and its representation of a corresponding ECM;
- The introduction of a novel physical-inspired model where the NN architecture approximates the ESP transfer functions referred to as the ohmic effects, the electrolyte diffusion and the non-uniform charge distribution in the cell;
- A comparison between the PI-ENNC model and its basic version using different training and test datasets available in the literature as well as different training procedures.

The paper is organized as follows: in Section 2 the BMS problem formulation is introduced; in Section 3 the BMS functioning is completely described explaining the KF application and its configuration settings; in Section 4, an in-depth description of the EMC and ENNC models are provided; Section 5 is dedicated to the PI-ENNC, which is the object of this paper. The manuscript continues with the dataset presentation, test settings and results commented in Sections 6–8, respectively. Finally, conclusions are drawn in Section 9. In Appendix A, additional figures regarding the predicted SoC and output voltage time series are provided.

2. Problem Formulation

An electrochemical cell can be formulated as a non-linear dynamic system described by the state equations:

$$\mathbf{x}[k+1] = \mathcal{F}(\mathbf{x}[k], \mathbf{u}[k]) \tag{1}$$

$$\mathbf{y}[k+1] = \mathcal{G}(\mathbf{x}[k], \mathbf{u}[k]) \tag{2}$$

where $\mathbf{x}$, $\mathbf{u}$ and $\mathbf{y}$ are respectively the cell state vector, the input and the output array and $\mathcal{F}$ and $\mathcal{G}$ are both non-linear functions. Equation (1) determines the cell state evolution whilst Equation (2) evaluates the output of the dynamic system.

As reported in many studies focused on the BMS generation through circuital models [8,51], the main physical quantities that contribute to the electrochemical cell state are the input current, the output voltage, the cell temperature and the State of Charge (SoC). According to [17], the terminal voltage of an electrochemical cell can be summarized as the superposition of three contributions:

- Quasi-stationary voltage V_{qst}: it corresponds to the OCV curve representing the voltage contribution related to the amount of charge actually stored in the cell. The use of the suffix quasi-stationary instead of OCV aims at distinguishing the manufacturer curve from the voltage contribution to predict while the cell is working, i.e. when the circuit is closed.
- Dynamic voltage contribution V_{dyn}: this contribution takes into account the voltage transient response due to the electrolyte diffusion phenomenon whose effects can be approximated to a low-pass filtering with respect to the input current [34].
- Instantaneous voltage contribution V_{ist}: it takes into account the internal resistance, namely the ohmic effects and the electrochemical kinetics of the cell as well [34]. Due to its nature, this contribution does not depend on previous battery states, i.e., it has no memory and it is mainly a function of the current.

According to the previous discussion, the terminal voltage of a battery cell can be formulated as follows:

$$V_{out}[k] = V_{qst}[k] + V_{dyn}[k] + V_{ist}[k] \tag{3}$$

Due to the non-linear electrochemical processes occurring during the charging/discharging phases, V_{dyn}, V_{qst} and V_{ist} may show non-linear dependencies with respect to the main physical quantities, i.e., the input current I_{in}, the state of charge SoC and the cell temperature T_{in}:

$$V_{dyn}[k] = \mathcal{F}_{dyn}\Big(V_{dyn}[k-1], SoC[k], I_{in}[k], T_{in}[k]\Big) \tag{4}$$

$$V_{ist}[k] = \mathcal{V}_{ist}(T_{in}[k], I_{in}[k], SoC[k]) = \mathcal{R}_{ist}(T_{in}[k], I_{in}[k])\, I_{in}[k] \tag{5}$$

$$V_{qst}[k] = \mathcal{V}_{qst}(SoC[k]) \tag{6}$$

where k is the time slot index.

In Equation (4), $\mathcal{F}_{dyn}$ addressed the non-linearities involved in the dynamic voltage contribution. As stated before, $\mathcal{F}_{dyn}$ has a low-pass filter behavior with respect to the input current I_{in}. In Equation (5), $\mathcal{R}_{ist}$ represents the resistance function that models the instantaneous voltage V_{ist}. It is supposed to approximate the ohmic effects involved in the cell, does not have memory and is only a function of the load current and the temperature.