Hochschule Offenburg University of Applied Sciences

Using neural ordinary differential equations for grey-box modelling of lithium-ion batteries

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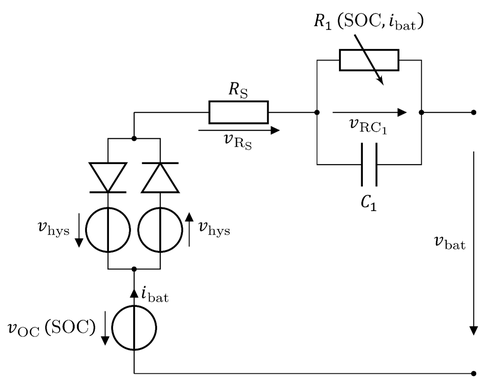
Motivation

- Growing demand for lithium-ion batteries in complex fields of application
  → Growing demand for battery models
- Parameterization of models is often time-demanding and complex
  → **New grey-box modelling approach using neural ordinary differential equations (NODEs)**
- Prismatic 180 Ah LFP/graphite cell (CALB CA180FI)

Battery Modelling

- Equivalent circuit model as a basis for grey-box modelling

$$\frac{\mathrm{d}SOC}{\mathrm{d}t} = -\frac{1}{C} i_{\mathrm{bat}}$$
$$\frac{\mathrm{d}v_{\mathrm{RC1}}}{\mathrm{d}t} = \frac{1}{C_1}\left(-\frac{1}{R_1(\mathrm{SOC}, i_{\mathrm{bat}})} v_{\mathrm{RC1}} + i_{\mathrm{bat}}\right)$$
$$v_{\mathrm{bat}} = v_{\mathrm{OC}}(\mathrm{SOC}) - v_{\mathrm{hys}} - R_{\mathrm{S}} i_{\mathrm{bat}} - v_{\mathrm{RC1}}$$



- Unknown parameters and dependencies are replaced by learnable parameters and neural networks:

$$\frac{\mathrm{d}SOC}{\mathrm{d}t} = -\frac{1}{\omega_0} i_{\mathrm{bat}} \quad (1)$$
$$\frac{\mathrm{d}v_{\mathrm{RC1}}}{\mathrm{d}t} = \frac{1}{\omega_1}\left(-\frac{1}{R_1(\mathrm{SOC}, i_{\mathrm{bat}})} v_{\mathrm{RC1}} + i_{\mathrm{bat}}\right) \quad (2)$$
$$R_1(\mathrm{SOC}, i_{\mathrm{bat}}) = \begin{cases} f(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_f), \forall i_{\mathrm{bat}} < 0 \\ g(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_g), \forall i_{\mathrm{bat}} > 0 \\ \frac{1}{2}\left(f(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_f) + g(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_g)\right), else \end{cases} \quad (3)$$
$$v_{\mathrm{bat}} = v_{\mathrm{OC}}(\mathrm{SOC}) - \omega_2 \cdot \mathrm{sgn}(i_{\mathrm{bat}}) - \omega_3 \cdot i_{\mathrm{bat}} - v_{\mathrm{RC1}} \quad (4)$$

- $f(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_f)$ and $g(\mathrm{SOC}, i_{\mathrm{bat}}, \boldsymbol{\theta}_g)$: feedforward networks with one hidden layer with 100 hidden neurons and rectified linear unit (ReLU) activation
- The differential equation (2) is a **neural ordinary differential equation**

Implementation and Training

- Python (version 3.7.6), PyTorch (version 1.9.0), torchdiffeq library (version 0.2.1)
- Differential equations solved with Dopri8
- Adam optimizer for loss minimization (MSE loss of true and learned battery voltage)

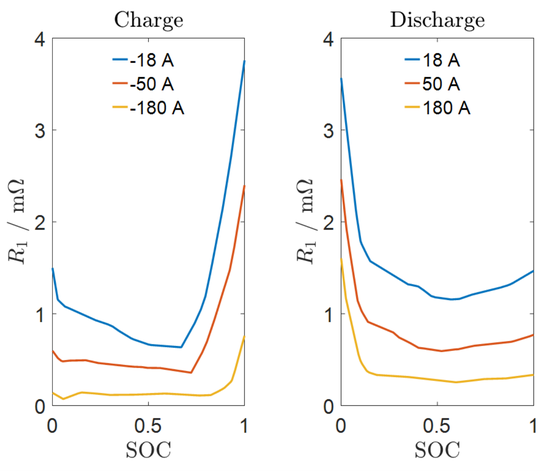
- Two training parts:
  1. Training of a static network:
     - the double-layer capacitance C_1 in eq. (2) was neglected
     - training data from constant current constant voltage charging and discharging
     - 300 epochs
  2. Pre-trained parameters were used for the dynamic modelling
     - the full grey-box model was used
     - training data from charging and discharging with current pulses
     - 30 epochs
- Test: synthetic load profile

Learned Parameters and Functions

The training process led to the following parameters:

$$C = \omega_0 = 191.50\ \mathrm{Ah}$$
$$C_1 = \omega_1 = 50.69\ \mathrm{kF}$$
$$v_{\mathrm{hys}} = \omega_2 = 11.25\ \mathrm{mV}$$
$$R_{\mathrm{S}} = \omega_3 = 281.4\ \mu\Omega$$

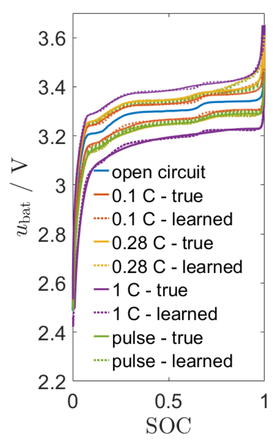
Resistance depends on SOC, absolute current, and sign of current (charge vs. discharge).



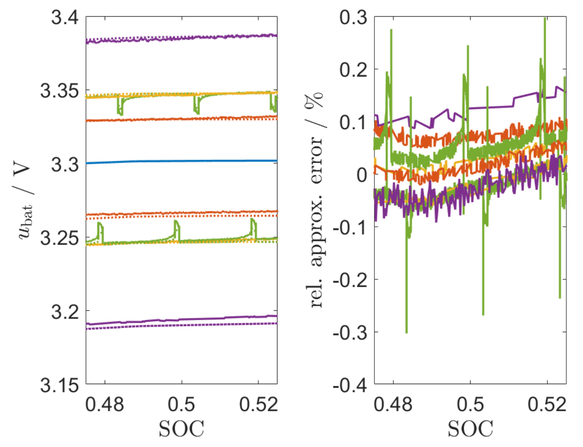
Results

Training data: CCCV charge/discharge curves at different C-rates + pulsed charge and discharge

Overview

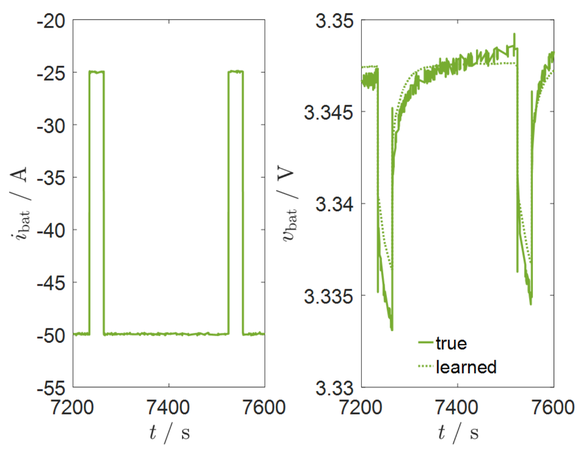


Zoom-In

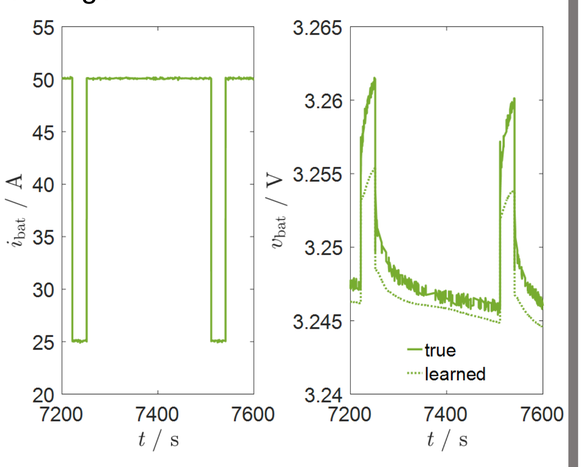


Training data: Pulsed charge and discharge

Charge

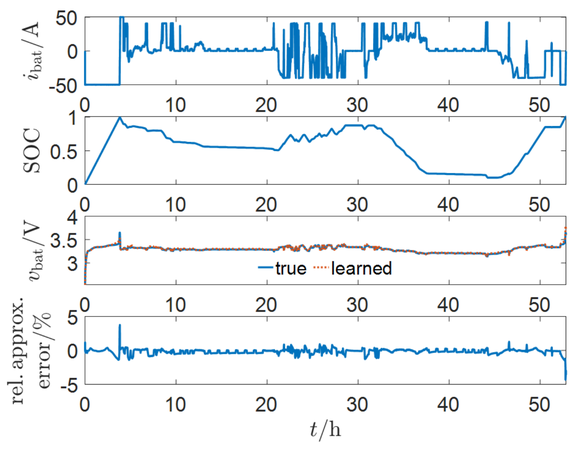


Discharge

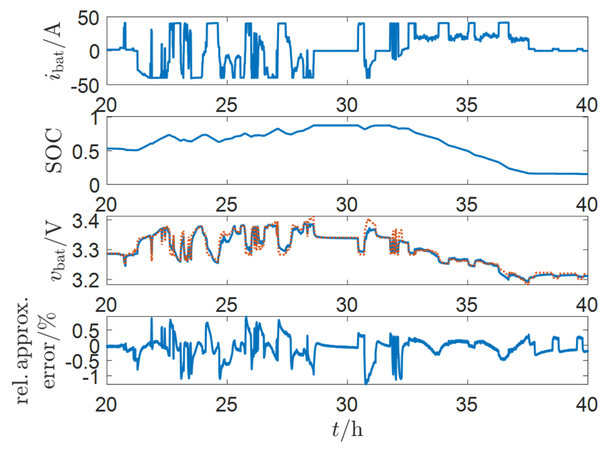


Test data: synthetic household profile over two days

Overview



Zoom-In



Conclusions

- Derivation of a grey-box model from a physics-based equivalent circuit model based on a coupling of physics-based ordinary differential equations and neural ordinary differential equations
- Reproduction of training data including fast dynamics with good accuracy
- Good agreement with experimental data for the test data set despite the small training database

References

- Brucker, J., Bessler, W.G. & Gasper, R. Grey-box modelling of lithium-ion batteries using neural ordinary differential equations. *Energy Inform* **4,** 15 (2021). https://doi.org/10.1186/s42162-021-00170-8.
- Brucker, J., Behmann, R., Bessler, W.G. & Gasper, R. Neural ordinary differential equations for grey-box modeling of lithium-ion batteries on the basis of an equivalent circuit model (2022). Manuscript submitted for publication.

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