

This Supplementary Note elucidates the mathematical calculation of the features in arbitrary cycles. Here we only use one cycle for demonstration of featurization..

For cut-off voltage features in the prior-cycling stage:

$$U_i = V(soc = soc_i)$$

$$soc_i = \{8, 20, 30, 40, 50, 61.1, 71.1, 81.1, 97\} \times 100\%$$

where,  $i = \{1, 2, \dots, 9\}$ ,  $V$  is battery voltage,  $soc$  is the state of charge, and  $soc_i$  is the accumulated state of charge at the  $i$ th charging step.

For inter-step voltage transient features and pseudo relaxation features in the in-cycling stage:

$$VC89 = V_9(start) - V_8(end)$$

where,  $V_9$  and  $V_8$  are the voltage vector in the ninth and eighth charging stage, respectively.  $start$  and  $end$  stand for the first and last voltage values in the vector, respectively.

$$VD9 = V_9(start) - \min(V_9)$$

where,  $V_9$  is the voltage vector in the ninth charging stage.  $\min$  is the minimum operator.

$$tVD9 = t(V = V_9(start)) - t(V = \min(V_9))$$

where,  $V_9$  is the voltage vector in the ninth charging stage,  $\min$  is the minimum operator,  $t$  is time and  $V$  is the battery voltage

For inter-step relaxation features in the in-cycling stage:

$$ReVC = V_9(end) - V_{re}(start)$$

where,  $V_9$  and  $V_{re}$  are the voltage vectors in the ninth charging stage rest stage, respectively.  $start$  and  $end$  stand for the first and last voltage values in the vector, respectively.

$$ReVD = V_{re}(start) - \min(V_{re})$$

where,  $V_{re}$  is the voltage vector in the rest stage.  $\min$  is the minimum operator.

$$tReVD = t(V = V_{re}(start)) - t(V = \min(V_{re}))$$

where,  $V_{re}$  is the voltage vector in the rest stage.  $\min$  is the minimum operator.  $t$  is time and  $V$  is the battery voltage

For intra-step voltage gradient features in the in-cycling stage:

$$Vg_i = \text{mean}(G(V_i))$$

where,  $i = \{1, 2, \dots, 9\}$ ,  $V_i$  is the voltage vector at the  $i$ th charging step,  $G$  is the gradient operator and  $\text{mean}$  is the mean operator.

For intra-step capacity features in the in-cycling stage:

$$Q_i = Q(soc = soc_i)$$

$$soc_i = \{8, 20, 30, 40, 50, 61.1, 71.1, 81.1, 97\} \times 100\%$$

where,  $i = \{1, 2, \dots, 9\}$ ,  $Q$  is battery charging capacity,  $soc$  is the state of charge, and  $soc_i$  is the accumulated state of charge at the  $i$ th charging step.

For lumped resistance features in the in-cycling stage:

$$RL_i = \frac{V_i(end) - V_i(start)}{I_i}$$

where,  $i = \{1, 2, \dots, 9\}$ ,  $V_i$  and  $I_i$  are the voltage vector and current value at the  $i$ th charging step, respectively.  $start$  and  $end$  stand for the first and last voltage values in the vector, respectively.

For ohmic resistance features in the in-cycling stage:

$$RO_i = \frac{V_{i+1}(start) - V_i(end)}{I_{i+1} - I_i}$$

where,  $i = \{1, 2, \dots, 8\}$ ,  $V_i$  and  $I_i$  are the voltage vector and current value at the  $i$ th charging step, respectively.  $start$  and  $end$  stand for the first and last voltage values in the vector, respectively.