

11576 lines (11576 loc) · 1.2 MB

LOW CURRENT OCV AT -10 degree celcius

In [1]:
 import pandas as pd

Read a specific sheet by name
 low_curr_ocv_minus_10= pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assig

low_curr_ocv_minus_10.head(10)

$\cap \cdot \cdot +$	11	
ou L	1 1	

נ[1]:		Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index	Cycle_Index	Cur
	0	1	3.010944	2012-06- 29 16:51:38	3.010944	1	1	0.
	1	2	3.026961	2012-06- 29 16:51:38	0.015765	2	1	1.
	2	3	8.035992	2012-06- 29 16:51:44	5.007575	3	1	0.
	3	4	13.043648	2012-06- 29 16:51:49	10.015231	3	1	0.
	4	5	18.051127	2012-06- 29 16:51:54	15.022710	3	1	0.
	5	6	23.058702	2012-06- 29 16:51:59	20.030285	3	1	0.
	6	7	28.066285	2012-06- 29 16:52:04	25.037868	3	1	0.
	7	8	33.073845	2012-06- 29 16:52:09	30.045427	3	1	0.
	8	9	38.081417	2012-06- 29 16:52:14	35.053000	3	1	0.
	9	10	43.089009	2012-06- 29 16:52:19	40.060591	3	1	0.
	4 (•

Out[2]:

	Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index
count	29785.00000	29785.000000	29785	29785.000000	29785.000000
mean	14893.00000	79452.354943	2012-06-30 14:55:48.690951936	36718.816502	5.960987
min	1.00000	3.010944	2012-06-29 16:51:38	0.015765	1.000000
25%	7447.00000	40580.632806	2012-06-30 04:07:57	18022.251663	5.000000
50%	14893.00000	77867.013967	2012-06-30 14:29:23	36665.442255	5.000000
75%	22339.00000	118452.093694	2012-07-01 01:45:49	55308.632827	7.000000
max	29785.00000	159037.139119	2012-07-01 13:02:14	76334.569682	8.000000
std	8598.33322	44515.946548	NaN	21570.964248	1.013849

In [3]:

low_curr_ocv_minus_10.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 29785 entries, 0 to 29784
Data columns (total 19 columns):

#	Column	Non-Null Count	Dtype
0	Data_Point	29785 non-null	int64
1	Test_Time(s)	29785 non-null	float64
2	Date_Time	29785 non-null	<pre>datetime64[ns]</pre>
3	<pre>Step_Time(s)</pre>	29785 non-null	float64
4	Step_Index	29785 non-null	int64
5	Cycle_Index	29785 non-null	int64
6	Current(A)	29785 non-null	float64
7	Voltage(V)	29785 non-null	float64
8	Charge_Capacity(Ah)	29785 non-null	float64
9	Discharge_Capacity(Ah)	29785 non-null	float64
10	Charge_Energy(Wh)	29785 non-null	float64
11	Discharge_Energy(Wh)	29785 non-null	float64
12	dV/dt(V/s)	29785 non-null	float64
13	<pre>Internal_Resistance(Ohm)</pre>	29785 non-null	int64
14	Is_FC_Data	29785 non-null	int64
15	AC_Impedance(Ohm)	29785 non-null	int64
16	ACI_Phase_Angle(Deg)	29785 non-null	int64
17	Temperature (C)_1	29785 non-null	float64
18	Temperature (C)_2	29785 non-null	float64
dtyp	es: datetime64[ns](1), floa	at64(11), int64(7)

LOW CURRENT OCV AT 0 degree celcius

memory usage: 4.3 MB

3.014942

min

1.000000

2012-06-18

11:49:18

0.031089

1.000000

```
2012-06-18
          25%
                7563.000000
                             41162.668955
                                                             17997.213788
                                                                              5.000000
                                                    23:15:18
                                                  2012-06-19
                                                             36930.843545
              15125.000000
                             79029.928468
                                                                              5.000000
                                                    09:46:26
                                                  2012-06-19
          75%
               22687.000000 120193.073943
                                                             55864.473308
                                                                              7.000000
                                                    21:12:29
                                                  2012-06-20
               30249.000000
                            161359.267642
                                                             76186.533244
                                                                              8.000000
                                                    08:38:36
                8732.278483
                             45209.697396
                                                            21853.017650
                                                                              1.030102
           std
                                                       NaN
In [7]:
         low curr ocv 0.info()
       <class 'pandas.core.frame.DataFrame'>
       RangeIndex: 30249 entries, 0 to 30248
       Data columns (total 19 columns):
            Column
                                      Non-Null Count Dtype
        0
            Data Point
                                      30249 non-null int64
            Test_Time(s)
                                      30249 non-null float64
        1
        2
            Date_Time
                                      30249 non-null datetime64[ns]
        3
            Step Time(s)
                                      30249 non-null float64
                                      30249 non-null int64
        4
            Step_Index
        5
            Cycle_Index
                                      30249 non-null int64
        6
            Current(A)
                                      30249 non-null float64
        7
            Voltage(V)
                                      30249 non-null float64
           Charge_Capacity(Ah)
                                     30249 non-null float64
            Discharge_Capacity(Ah) 30249 non-null float64
        10 Charge_Energy(Wh)
                                      30249 non-null float64
        11 Discharge_Energy(Wh)
                                      30249 non-null float64
        12 dV/dt(V/s)
                                      30249 non-null float64
        13 Internal_Resistance(Ohm) 30249 non-null int64
        14 Is FC Data
                                      30249 non-null int64
        15 AC_Impedance(Ohm)
                                      30249 non-null int64
        16 ACI Phase Angle(Deg)
                                      30249 non-null
                                                      int64
            Temperature (C) 1
                                      30249 non-null
                                                      float64
        17
        18 Temperature (C)_2
                                      30249 non-null float64
       dtypes: datetime64[ns](1), float64(11), int64(7)
```

LOW CURRENT OCV AT 10 degree celcius

memory usage: 4.4 MB

```
In [8]: low_curr_ocv_10=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\
In [9]: low_curr_ocv_10.head(10)

Out[9]: Data_Point Test_Time(s) Date_Time Step_Time(s) Step_Index Cycle_Index Cur

2012-06-
1 3.014079 11 3.014079 1 0
```

			18:47:47				
1	2	3.025053	2012-06- 11 18:47:47	0.000002	2	1	1.
2	3	8.032849	2012-06- 11 18:47:52	5.007554	3	1	0.
3	4	13.040499	2012-06- 11 18:47:57	10.015204	3	1	0.
4	5	18.046321	2012-06- 11 18:48:02	15.021026	3	1	0.
5	6	23.053825	2012-06- 11 18:48:07	20.028530	3	1	0.
6	7	28.061527	2012-06- 11 18:48:12	25.036233	3	1	0.
7	8	33.068989	2012-06- 11 18:48:17	30.043694	3	1	0.
8	9	38.076571	2012-06- 11 18:48:22	35.051276	3	1	0.
9	10	43.084085	2012-06- 11 18:48:27	40.058790	3	1	0.

In [10]:

low_curr_ocv_10.describe()

Out[10]:

	Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index
count	31898.00000	31898.000000	31898	31898.000000	31898.000000
mean	15949.50000	84407.542774	2012-06-12 23:21:28.604269824	35034.642104	5.807605
min	1.00000	3.014079	2012-06-11 18:47:47	0.000002	1.000000
25%	7975.25000	43127.482188	2012-06-12 12:56:42.249999872	14612.052933	5.000000
50%	15949.50000	83059.113340	2012-06-13 00:02:14.500000	34527.490563	5.000000
75%	23923.75000	126287.349589	2012-06-13 12:02:42.750000128	54492.820953	7.000000
max	31898.00000	169513.642825	2012-06-14 00:03:10	75041.088878	8.000000

```
9208.30378 47856.153587
                                                         NaN 22318.590732
In [11]:
          low_curr_ocv_10.info()
        <class 'pandas.core.frame.DataFrame'>
        RangeIndex: 31898 entries, 0 to 31897
        Data columns (total 19 columns):
                                        Non-Null Count Dtype
        --- -----
                                        31898 non-null int64
         0
             Data_Point
         1
             Test_Time(s)
                                        31898 non-null float64
           Date_Time
         2
                                       31898 non-null datetime64[ns]
         3
            Step Time(s)
                                       31898 non-null float64
                                       31898 non-null int64
            Step_Index
         5
            Cycle_Index
                                       31898 non-null int64
                                       31898 non-null float64
            Current(A)
         6
           Voltage(V) 31898 non-null float64
Charge_Capacity(Ah) 31898 non-null float64
         7
         9 Discharge_Capacity(Ah) 31898 non-null float64
         10 Charge_Energy(Wh) 31898 non-null float64
11 Discharge_Energy(Wh) 31898 non-null float64
12 dV/dt(V/s) 31898 non-null float64
                                       31898 non-null float64
         12 dV/dt(V/s)
         13 Internal_Resistance(Ohm) 31898 non-null int64
         14 Is_FC_Data
                                       31898 non-null int64
         15 AC Impedance(Ohm)
                                       31898 non-null int64
         16 ACI_Phase_Angle(Deg)
                                       31898 non-null int64
         17
             Temperature (C)_1
                                       31898 non-null float64
                                        31898 non-null float64
         18 Temperature (C)_2
        dtypes: datetime64[ns](1), float64(11), int64(7)
        memory usage: 4.6 MB
```

LOW CURRENT OCV AT 20 degree celcius

In [12]:	low_curr	_ocv	_20=pd.read_e	excel(r"C:\l	Jsers\jaiku\P	ycharmProjeo	cts\Assignme	nts\
In [13]:	low_curr	_ocv_	_20.head(10)					
Out[13]:	Data_F	Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index	Cycle_Index	Cur
	0	1	3.007810	2012-06- 14 12:13:15	3.007810	1	1	0.
	1	2	3.008080	2012-06- 14 12:13:15	0.000002	2	1	1.
	2	3	8.015990	2012-06- 14 12:13:20	5.007662	3	1	0.
	3	4	13.023481	2012-06-	10.015153	3	1	0.

			12:13:25				
4	5	18.035039	2012-06- 14 12:13:30	15.026711	3	1	0.
5	6	23.042624	2012-06- 14 12:13:35	20.034296	3	1	0.
6	7	28.050181	2012-06- 14 12:13:40	25.041853	3	1	0.
7	8	33.057714	2012-06- 14 12:13:45	30.049386	3	1	0.
8	9	38.065421	2012-06- 14 12:13:50	35.057093	3	1	0.
9	10	43.072973	2012-06- 14 12:13:55	40.064645	3	1	0.

In [14]:

low_curr_ocv_20.describe()

Out[14]:

	Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index
count	31018.000000	31018.000000	31018	31018.000000	31018.000000
mean	15509.500000	82530.938666	2012-06-15 11:08:43.815655168	37436.752180	5.955671
min	1.000000	3.007810	2012-06-14 12:13:15	0.000002	1.000000
25%	7755.250000	42125.027738	2012-06-14 23:55:17.249999872	17983.441759	5.000000
50%	15509.500000	80954.993049	2012-06-15 10:42:27.500000	37399.049136	5.000000
75%	23263.750000	123082.373990	2012-06-15 22:24:35.750000128	56814.656519	7.000000
max	31018.000000	165211.592285	2012-06-16 10:06:45	76708.858391	8.000000
std	8954.269661	46356.820098	NaN	22362.338814	1.053492
4					•

In [15]:

low_curr_ocv_20.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 31018 entries, 0 to 31017
Data columns (total 19 columns):

Column Non-Null Count Dtype

```
Data Point
                              31018 non-null int64
    Test_Time(s)
1
                              31018 non-null float64
2
    Date_Time
                              31018 non-null datetime64[ns]
3
    Step_Time(s)
                             31018 non-null float64
    Step_Index
                              31018 non-null int64
5
    Cycle_Index
                              31018 non-null int64
6
                              31018 non-null float64
    Current(A)
7
    Voltage(V)
                              31018 non-null
                                             float64
8
    Charge_Capacity(Ah)
                             31018 non-null float64
9
    Discharge_Capacity(Ah) 31018 non-null float64
10 Charge_Energy(Wh)
                              31018 non-null float64
11 Discharge_Energy(Wh)
                              31018 non-null float64
    dV/dt(V/s)
                              31018 non-null
                                             float64
13
    Internal_Resistance(Ohm) 31018 non-null int64
14
    Is_FC_Data
                              31018 non-null int64
15 AC_Impedance(Ohm)
                              31018 non-null int64
   ACI_Phase_Angle(Deg)
                             31018 non-null int64
    Temperature (C)_1
                              31018 non-null float64
17
                              31018 non-null float64
    Temperature (C)_2
dtypes: datetime64[ns](1), float64(11), int64(7)
```

LOW CURRENT OCV AT 25 degree celcius

memory usage: 4.5 MB

In [16]: low_curr_ocv_25=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\ In [17]: low_curr_ocv_25.head(10) Out[17]: Data_Point Test_Time(s) Date_Time Step_Time(s) Step_Index Cycle_Index Cur 2012-09-0 3.003881 05 3.003881 0. 09:50:31 2012-09-1 8.004174 05 5.000008 1. 09:50:36 2012-09-2 3 2 13.004248 05 10.000082 1. 09:50:41 2012-09-3 18.004260 15.000093 1. 05 09:50:46 2012-09-23.005579 05 20.001413 1. 09:50:51 2012-09-28.005657 05 25.001492 1. 09:50:56 2012-09-33.011929 05 30.007763 ∩0.51.∩1

7	8	38.011951	2012-09- 05 09:51:06	35.007785	2	1	1.
8	9	43.011997	2012-09- 05 09:51:11	40.007831	2	1	1.
9	10	48.012036	2012-09- 05 09:51:16	45.007870	2	1	1.

In [18]:

low_curr_ocv_25.describe()

Out[18]:

	Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index
count	32307.00000	32307.000000	32307	32307.000000	32307.000000
mean	16154.00000	85506.863991	2012-09-06 09:35:35.959884800	36302.546619	5.837713
min	1.00000	3.003881	2012-09-05 09:50:31	3.003881	1.000000
25%	8077.50000	43696.841249	2012-09-05 21:58:45.500000	15874.938811	5.000000
50%	16154.00000	84091.821468	2012-09-06 09:12:01	36076.586865	5.000000
75%	24230.50000	127800.461601	2012-09-06 21:20:30.500000	56272.784453	7.000000
max	32307.00000	171495.535618	2012-09-07 09:28:46	76592.209924	8.000000
std	9326.37191	48357.812231	NaN	22968.249246	1.217815

In [19]: low_curr_ocv_25.info()

<class 'pandas.core.frame.DataFrame'> RangeIndex: 32307 entries, 0 to 32306 Data columns (total 18 columns):

#	Column	Non-Null Count	Dtype
0	Data_Point	32307 non-null	int64
1	Test_Time(s)	32307 non-null	float64
2	Date_Time	32307 non-null	<pre>datetime64[ns]</pre>
3	<pre>Step_Time(s)</pre>	32307 non-null	float64
4	Step_Index	32307 non-null	int64
5	Cycle_Index	32307 non-null	int64
6	Current(A)	32307 non-null	float64
7	Voltage(V)	32307 non-null	float64
8	Charge_Capacity(Ah)	32307 non-null	float64
9	Discharge_Capacity(Ah)	32307 non-null	float64
10	Charge_Energy(Wh)	32307 non-null	float64
11	Discharge_Energy(Wh)	32307 non-null	float64

```
12 dV/dt(V/s)
                          32307 non-null float64
13 Internal_Resistance(Ohm) 32307 non-null int64
14 Is_FC_Data
                          32307 non-null int64
```

15 AC_Impedance(Ohm) 32307 non-null int64 16 ACI_Phase_Angle(Deg) 32307 non-null int64 17 Temperature (C)_1 32307 non-null float64

dtypes: datetime64[ns](1), float64(10), int64(7)

memory usage: 4.4 MB

LOW CURRENT OCV AT 30 degree celcius



ut[21]:		Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index	Cycle_Index	Cur
	0	1	3.010808	2012-06- 25 10:58:13	3.010808	1	1	0.
	1	2	3.041952	2012-06- 25 10:58:13	0.030896	2	1	1
	2	3	8.057809	2012-06- 25 10:58:18	5.015575	3	1	0.
	3	4	13.065362	2012-06- 25 10:58:23	10.023128	3	1	0.
	4	5	18.072954	2012-06- 25 10:58:28	15.030720	3	1	0.
	5	6	23.080509	2012-06- 25 10:58:33	20.038275	3	1	0.
	6	7	28.088092	2012-06- 25 10:58:38	25.045859	3	1	0.
	7	8	33.095648	2012-06- 25 10:58:43	30.053414	3	1	0.
	8	9	38.103228	2012-06- 25 10:58:48	35.060994	3	1	0.
	9	10	43.110795	2012-06- 25 10:58:53	40.068561	3	1	0.

In [22]: low_curr_ocv_30.describe() Out[22]: **Data Point** Test Time(s) **Date Time** Step Time(s) Step Index count 31150.000000 31150.000000 31150 31150.000000 31150.000000 2012-06-26 15575.500000 82879.119805 37868.880320 5.967159 mean 09:59:30.199871488 2012-06-25 min 1.000000 3.010808 0.030896 1.000000 10:58:13 2012-06-25 25% 7788.250000 42289.364036 18343.988166 5.000000 22:43:00.249999872 2012-06-26 50% 37842.221660 15575.500000 81284.579150 5.000000 09:32:55.500000 2012-06-26 57340.455169 23362.750000 123576.509714 7.000000 21:17:47.750000128 2012-06-27 8.000000 31150.000000 165868.338984 77269.004464 09:02:40 8992.374779 46527.087207 NaN 22474.828502 1.040072 In [23]: low_curr_ocv_30.info() <class 'pandas.core.frame.DataFrame'> RangeIndex: 31150 entries, 0 to 31149 Data columns (total 19 columns): Column # Non-Null Count Dtype ---_____ _____ ____ 0 Data Point 31150 non-null int64 Test_Time(s) 31150 non-null float64 1 2 Date Time 31150 non-null datetime64[ns] 3 Step_Time(s) 31150 non-null float64 4 Step_Index 31150 non-null int64 5 Cycle Index 31150 non-null int64 Current(A) 31150 non-null float64 6 7 31150 non-null float64 Voltage(V) 8 Charge_Capacity(Ah) 31150 non-null float64 9 Discharge Capacity(Ah) 31150 non-null float64 10 Charge_Energy(Wh) 31150 non-null float64 11 Discharge_Energy(Wh) 31150 non-null float64 12 dV/dt(V/s)31150 non-null float64 13 Internal_Resistance(Ohm) 31150 non-null int64 14 Is FC Data 31150 non-null int64 AC Impedance(Ohm) 15 31150 non-null int64 16 ACI_Phase_Angle(Deg) 31150 non-null int64 17 Temperature (C) 1 31150 non-null float64 18 Temperature (C) 2 31150 non-null float64 dtypes: datetime64[ns](1), float64(11), int64(7) memory usage: 4.5 MB

LOW CURRENT OCV AT 40 degree

ceicius

	1								D
[25]:	low_c	urr_ocv_	_40.hea	d(10)					
[25]:	Dat	ta_Point	Test_Ti	me(s)	Date_Time	Step_Time(s)	Step_Index	Cycle_Index	C
	0	1	3.0	10283	2012-06- 27 11:43:25	3.010283	1	1	
	1	2	3.0	26131	2012-06- 27 11:43:25	0.015609	2	1	
	2	3	8.0	33910	2012-06- 27 11:43:30	5.007549	3	1	
	3	4	13.0	41500	2012-06- 27 11:43:35	10.015140	3	1	
	4	5	18.0	49071	2012-06- 27 11:43:40	15.022711	3	1	
	5	6	23.0	56643	2012-06- 27 11:43:45	20.030282	3	1	
	6	7	28.0	64215	2012-06- 27 11:43:50	25.037854	3	1	
	7	8	33.0	71785	2012-06- 27 11:43:55	30.045425	3	1	
	8	9	38.0	79286	2012-06- 27 11:44:00	35.052926	3	1	
	9	10	43.0	86932	2012-06- 27 11:44:05	40.060571	3	1	
	1								
[26]:	low_c	urr_ocv_	_40.des	cribe()				
[26]:		Data_	Point	Test_	Time(s)	Date_Time	e Step_Time	e(s) Step_I	nde
	count	31258.0	00000	31258	3.000000	31258	31258.0000	000 31258.00	000
	mean	15629.5	00000	83182		2012-06-28	3 38403.6742	272 5.98	

```
2012-06-27
                    1.000000
                                  3.010283
                                                                 0.015609
                                                                              1.000000
           min
                                                    11:43:25
                                                 2012-06-27
           25%
                 7815.250000
                              42427.009169
                                                             18823.463111
                                                                              5.000000
                                           23:30:30.249999872
                                                  2012-06-28
           50%
               15629.500000
                              81557.428742
                                                             38388.046949
                                                                              5.000000
                                              10:22:40.500000
                                                  2012-06-28
                23443.750000 123985.717499
                                                             57952.630847
                                                                              7.000000
                                           22:09:49.750000128
                                                  2012-06-29
                                                             77785.938692
                                                                              8.000000
           max 31258.000000 166414.916638
                                                    09:56:59
                                                            22568.608281
                 9023.551694
                              46653.945691
                                                       NaN
                                                                              1.019973
In [27]:
          low_curr_ocv_40.info()
        <class 'pandas.core.frame.DataFrame'>
        RangeIndex: 31258 entries, 0 to 31257
        Data columns (total 19 columns):
             Column
                                       Non-Null Count Dtype
                                       -----
         0
            Data_Point
                                      31258 non-null int64
            Test Time(s)
                                      31258 non-null float64
           Date Time
                                     31258 non-null datetime64[ns]
         2
                                      31258 non-null float64
         3
            Step_Time(s)
         4
            Step_Index
                                      31258 non-null int64
         5
            Cycle_Index
                                      31258 non-null int64
            Current(A)
                                     31258 non-null float64
         7
            Voltage(V)
                                     31258 non-null float64
            Charge_Capacity(Ah) 31258 non-null float64
         8
            Discharge_Capacity(Ah) 31258 non-null float64
         9
         10 Charge_Energy(Wh)
                                      31258 non-null float64
                                     31258 non-null float64
         11 Discharge_Energy(Wh)
         12 dV/dt(V/s)
                                      31258 non-null float64
         13 Internal_Resistance(Ohm) 31258 non-null int64
         14 Is FC Data
                                      31258 non-null int64
         15 AC Impedance(Ohm)
                                       31258 non-null int64
```

dtypes: datetime64[ns](1), float64(11), int64(7)
memory usage: 4.5 MB

16 ACI_Phase_Angle(Deg)

17 Temperature (C)_1 18 Temperature (C) 2

LOW CURRENT OCV AT 50 degree celcius

31258 non-null int64 31258 non-null float64

31258 non-null float64

```
In [28]: low_curr_ocv_50=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\
In [29]: low_curr_ocv_50.head(10)

Out[29]: Data_Point Test_Time(s) Date_Time Step_Time(s) Step_Index Cycle_Index Cur
```

0	1	3.008714	2012-07- 02 10:52:00	3.008714	1	1	0.
1	2	3.020297	2012-07- 02 10:52:00	0.000002	2	1	1.
2	3	8.037763	2012-07- 02 10:52:05	5.007566	3	1	0.
3	4	13.045325	2012-07- 02 10:52:10	10.015128	3	1	0.
4	5	18.052910	2012-07- 02 10:52:15	15.022712	3	1	0.
5	6	23.060484	2012-07- 02 10:52:20	20.030287	3	1	0.
6	7	28.068046	2012-07- 02 10:52:25	25.037848	3	1	0.
7	8	33.075622	2012-07- 02 10:52:30	30.045425	3	1	0.
8	9	38.083297	2012-07- 02 10:52:35	35.053100	3	1	0.
9	10	43.090758	2012-07- 02 10:52:40	40.060561	3	1	0.

In [30]: low_curr_ocv_50.describe()

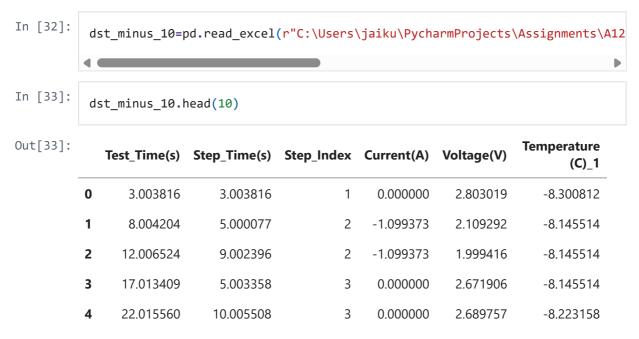
Out[30]:

	Data_Point	Test_Time(s)	Date_Time	Step_Time(s)	Step_Index
count	31475.000000	31475.000000	31475	31475.000000	31475.000000
mean	15738.000000	83704.689997	2012-07-03 10:07:02.332041216	38368.988081	5.975473
min	1.000000	3.008714	2012-07-02 10:52:00	0.000002	1.000000
25%	7869.500000	42695.210585	2012-07-02 22:43:32.500000	18645.694362	5.000000
50%	15738.000000	82097.290906	2012-07-03 09:40:15	38347.986437	5.000000
75%	23606.500000	124794.372180	2012-07-03 21:31:52.500000	58047.774699	7.000000

```
2012-07-04
          max 31475.000000 167494.127364
                                                           77843.159249
                                                                            8.000000
                                                   09:23:33
           std
                9086.194198
                             46988.606063
                                                      NaN
                                                           22713.080086
                                                                            1.035112
In [31]:
          low_curr_ocv_50.info()
        <class 'pandas.core.frame.DataFrame'>
       RangeIndex: 31475 entries, 0 to 31474
       Data columns (total 19 columns):
            Column
                                      Non-Null Count Dtype
            -----
        0
            Data_Point
                                      31475 non-null int64
        1
           Test_Time(s)
                                     31475 non-null float64
        2
           Date Time
                                     31475 non-null datetime64[ns]
        3
           Step_Time(s)
                                     31475 non-null float64
        4
            Step Index
                                     31475 non-null int64
        5
           Cycle Index
                                     31475 non-null int64
        6
           Current(A)
                                     31475 non-null float64
        7
            Voltage(V)
                                     31475 non-null float64
        8
            Charge_Capacity(Ah)
                                    31475 non-null float64
            Discharge_Capacity(Ah) 31475 non-null float64
        9
        10 Charge_Energy(Wh)
                                      31475 non-null float64
        11 Discharge_Energy(Wh)
                                    31475 non-null float64
        12 dV/dt(V/s)
                                     31475 non-null float64
        13 Internal Resistance(Ohm) 31475 non-null int64
        14 Is FC Data
                                     31475 non-null int64
        15 AC_Impedance(Ohm)
                                     31475 non-null int64
        16 ACI_Phase_Angle(Deg)
                                      31475 non-null int64
            Temperature (C)_1
                                      31475 non-null float64
        17
        18 Temperature (C)_2
                                     31475 non-null float64
        dtypes: datetime64[ns](1), float64(11), int64(7)
       memory usage: 4.6 MB
```

DYNAMIC TEST PROFILES

Dynamic test profile at -10 degree celcius



Dynamic test profile at 10 degree celcius

In [40]: dst 10=pd.read excel(r"C:\Users\jaiku\PycharmProjects\Assignments\A123 batt

In [41]: dst 10.head(10) Out[41]: **Temperature** Test_Time(s) Step_Time(s) Step_Index Current(A) Voltage(V) $(C)_1$ 0 3.008291 3.008291 1 0.000000 2.968602 9.646121 1 8.015758 5.007161 2 -1.099185 2.729152 9.690903 2 13.018937 10.010341 2 -1.099373 2.703299 9.598107 3 18.027239 15.018642 2 -1.099373 2.678369 9.797547 23.031320 2 -1.099373 4 20.022724 2.654363 9.766615 5 2 -1.099373 28.035736 25.027140 2.629125 9.721836 6 33.039112 30.030516 2 -1.099373 2.603272 9.797547 7 38.047386 35.038790 2 -1.099373 2.576496 9.690903 8 43.053577 40.044981 2 -1.099373 2.547873 9.918034 9 48.062643 45.054046 2 -1.099373 2.515864 9.873258 In [42]: dst_10.describe() Out[42]: Tem Test_Time(s) Step_Time(s) Step_Index Current(A) Voltage(V) 23881.000000 2.388100e+04 23881.000000 23881.000000 23881.000000 2388 19919.260228 4.755559e+02 15.518613 -0.356659 3.190354 1 mean 10203.319502 4.779053e+02 6.705619 0.932044 0.224014 std 3.008291 7.699193e-07 1.000000 -3.849407 1.987413 min 25% 10199.540085 8.000000 3.077862 1.497195e+02 -0.848430 1 50% 20191.833861 16.000000 -0.243238 3.196048 3.095074e+02 1 30156.128886 5.997450e+02 **75%** 24.000000 0.072130 3.302231 1 36435.385542 2.681824e+03 27.000000 2.061261 3.699877 1 max In [43]: dst_10.info() <class 'pandas.core.frame.DataFrame'> RangeIndex: 23881 entries, 0 to 23880 Data columns (total 6 columns): # Column Non-Null Count Dtype ---0 Test_Time(s) float64 23881 non-null 1 23881 non-null float64 Step_Time(s) 2 Step_Index 23881 non-null int64 3 Current(A) 23881 non-null float64 Voltage(V) 23881 non-null float64

5 Temperature (C)_1 23881 non-null float64

memory usage: 1.1 MB

dtypes: float64(5), int64(1)

Dynamic test profile at 20 degree celcius

In [44]:
 dst_20=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\A123 batt

In [45]:

dst_20.head(10)

Out[45]:

Test_Time(s)	Step_Time(s)	Step_Index	Current(A)	Voltage(V)	Temperature (C)_1
3.008332	3.008332	1	0.000000	3.108637	18.427523
8.014952	5.006227	2	-1.099776	2.891659	18.444551
13.018221	10.009497	2	-1.099776	2.877501	18.427523
18.022437	15.013712	2	-1.099957	2.864575	18.489090
23.026696	20.017971	2	-1.099776	2.851957	18.382978
28.035930	25.027205	2	-1.099957	2.839954	18.458305
33.045322	30.036597	2	-1.099776	2.827950	18.365955
38.051520	35.042795	2	-1.099957	2.815948	18.427523
43.066605	40.057881	2	-1.099776	2.803944	18.352194
48.077106	45.068381	2	-1.099776	2.791941	18.321405
	3.008332 8.014952 13.018221 18.022437 23.026696 28.035930 33.045322 38.051520 43.066605	3.008332 3.008332 8.014952 5.006227 13.018221 10.009497 18.022437 15.013712 23.026696 20.017971 28.035930 25.027205 33.045322 30.036597 38.051520 35.042795 43.066605 40.057881	3.008332 3.008332 1 8.014952 5.006227 2 13.018221 10.009497 2 18.022437 15.013712 2 23.026696 20.017971 2 28.035930 25.027205 2 33.045322 30.036597 2 38.051520 35.042795 2 43.066605 40.057881 2	3.008332 3.008332 1 0.000000 8.014952 5.006227 2 -1.099776 13.018221 10.009497 2 -1.099776 18.022437 15.013712 2 -1.099957 23.026696 20.017971 2 -1.099776 28.035930 25.027205 2 -1.099957 33.045322 30.036597 2 -1.099776 38.051520 35.042795 2 -1.099957 43.066605 40.057881 2 -1.099776	3.008332 3.008332 1 0.000000 3.108637 8.014952 5.006227 2 -1.099776 2.891659 13.018221 10.009497 2 -1.099776 2.877501 18.022437 15.013712 2 -1.099957 2.864575 23.026696 20.017971 2 -1.099776 2.851957 28.035930 25.027205 2 -1.099957 2.839954 33.045322 30.036597 2 -1.099776 2.827950 38.051520 35.042795 2 -1.0999776 2.815948 43.066605 40.057881 2 -1.099776 2.803944

In [46]:

dst 20.describe()

Out[46]:

	Test_Time(s)	Step_Time(s)	Step_Index	Current(A)	Voltage(V)	Tem
count	24992.000000	2.499200e+04	24992.000000	24992.000000	24992.000000	2499
mean	20478.506604	4.711195e+02	15.573944	-0.362114	3.195718	2
std	10524.199546	4.800529e+02	6.722357	0.935984	0.229664	
min	3.008332	7.699193e-07	1.000000	-3.849713	1.898483	1
25%	10446.853748	1.524163e+02	8.000000	-0.862705	3.091094	1
50%	20715.938621	3.099327e+02	16.000000	-0.279794	3.208663	1
75%	30962.624857	5.888735e+02	24.000000	0.063971	3.315767	2
max	37521.292897	2.867548e+03	27.000000	2.061054	3.732181	2

In [47]:

dst_20.info()

<class 'pandas.core.frame.DataFrame'>

```
RangeIndex: 24992 entries, 0 to 24991
```

Data columns (total 6 columns): # Column Non-Null Count Dtyne

#	COTUMN	Non-Null Count	Dtype
0	Test_Time(s)	24992 non-null	float64
1	<pre>Step_Time(s)</pre>	24992 non-null	float64
2	Step_Index	24992 non-null	int64
3	Current(A)	24992 non-null	float64
4	Voltage(V)	24992 non-null	float64
5	Temperature (C)_1	24992 non-null	float64

dtypes: float64(5), int64(1)

memory usage: 1.1 MB

Dynamic test profile at 25 degree celcius

In [48]: dst_25=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\A123 batt In [49]: dst 25.head(10)

Out[49]:

	Test_Time(s)	Step_Time(s)	Step_Index	Current(A)	Voltage(V)	Temperature (C)_1
0	3.053504	3.000204	1	0.000000	2.766393	26.788187
1	8.061154	5.007273	2	-1.099373	2.501398	26.818743
2	13.062293	10.008411	2	-1.099185	2.435226	26.818743
3	18.071620	15.017739	2	-1.099373	2.340432	26.713451
4	23.073773	20.019892	2	-1.099185	2.115448	26.788187
5	24.301853	21.247971	2	-1.099373	1.998801	26.893473
6	29.307341	5.004141	3	0.000000	2.460464	26.893473
7	34.311587	10.008388	3	0.000000	2.474314	26.713451
8	39.319818	15.016618	3	0.000000	2.482316	26.818743
9	44.325095	20.021896	3	0.000000	2.486933	26.937641

In [50]: dst_25.describe()

Out[50]:

	Test_Time(s)	Step_Time(s)	Step_Index	Current(A)	Voltage(V)	Tem
count	24469.000000	2.446900e+04	24469.000000	24469.000000	24469.000000	2446
mean	19726.353242	4.718362e+02	15.557767	-0.363447	3.204312	2
std	10192.971787	5.018513e+02	6.710170	0.942908	0.211759	
min	3.053504	3.849596e-07	1.000000	-3.849407	1.937861	2
25%	10017.592323	1.497245e+02	8.000000	-0.867589	3.110487	2
50%	19958.708627	3.061075e+02	16.000000	-0.286440	3.214515	2
75%	29860.944817	5.805784e+02	24.000000	0.060672	3.311772	2

```
max 36294.795004 3.070756e+03
                                              27.000000
                                                            2.061261
                                                                         3.699877
                                                                                      2
In [51]:
          dst_25.info()
        <class 'pandas.core.frame.DataFrame'>
        RangeIndex: 24469 entries, 0 to 24468
        Data columns (total 6 columns):
             Column
                                Non-Null Count
         0
             Test_Time(s)
                                24469 non-null float64
         1
             Step_Time(s)
                                24469 non-null float64
         2
             Step_Index
                                24469 non-null int64
         3
             Current(A)
                                24469 non-null float64
         4
             Voltage(V)
                                24469 non-null float64
             Temperature (C)_1 24469 non-null float64
        dtypes: float64(5), int64(1)
        memory usage: 1.1 MB
```

Dynamic test profile at 30 degree celcius

```
In [52]:
           dst_30=pd.read_excel(r"C:\Users\jaiku\PycharmProjects\Assignments\A123 batt
In [53]:
           dst 30.head(10)
Out[53]:
                                                                               Temperature
              Test_Time(s) Step_Time(s) Step_Index Current(A) Voltage(V)
                                                                                       (C) 1
                 3.004871
                                3.004871
                                                        0.000000
                                                                     3.075400
                                                                                  31.391201
           1
                 8.011347
                                5.006164
                                                        -1.099373
                                                                     2.888580
                                                                                  31.242373
          2
                13.017574
                               10.012391
                                                   2
                                                        -1.099373
                                                                     2.876269
                                                                                  31.391201
                                                                                  31.421654
          3
                18.023831
                               15.018647
                                                   2
                                                        -1.099373
                                                                     2.864882
           4
                23.027999
                               20.022816
                                                   2
                                                        -1.099373
                                                                                  31.496058
                                                                     2.853494
          5
                28.032410
                                                   2
                                                        -1.099373
                               25.027227
                                                                     2.842414
                                                                                  31.421654
           6
                33.039675
                                                   2
                                                        -1.099373
                               30.034492
                                                                     2.831334
                                                                                  31.421654
          7
                                                   2
                38.041781
                               35.036597
                                                        -1.099373
                                                                     2.819946
                                                                                  31.465605
           8
                43.043244
                               40.038061
                                                   2
                                                        -1.099373
                                                                                  31.465605
                                                                     2.808558
                                                   2
                48.043298
                               45.038114
                                                        -1.099560
                                                                     2.796555
                                                                                  31.391201
In [54]:
           dst_30.describe()
Out[54]:
                                                                                            Tem
                   Test_Time(s)
                                 Step_Time(s)
                                                  Step_Index
                                                                Current(A)
                                                                               Voltage(V)
           count 24598.000000 2.459800e+04 24598.000000 24598.000000
                                                                             24598.000000
                                                                                           2459
```

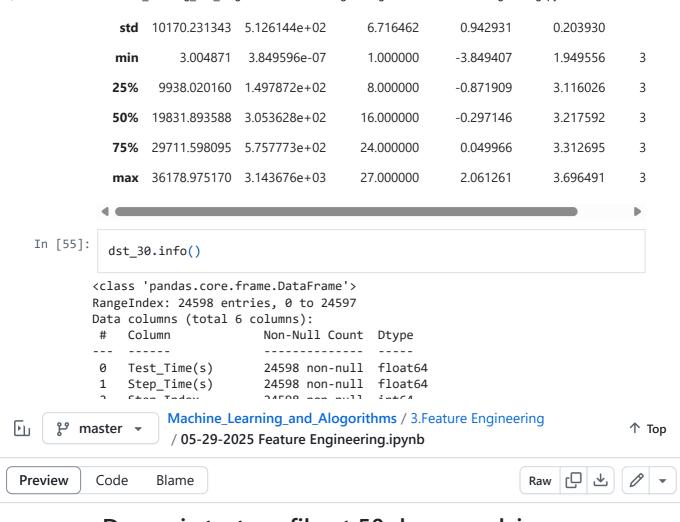
15.567973

-0.364780

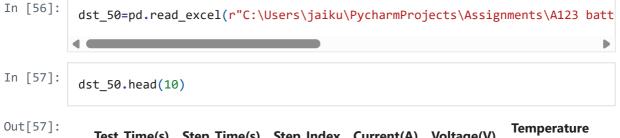
3.206956

19621.906470 4.721762e+02

3



Dynamic test profile at 50 degree celcius



	Test_Time(s)	Step_Time(s)	Step_Index	Current(A)	Voltage(V)	(C)_1
0	3.007451	3.007451	1	0.000000	2.775626	50.789497
1	8.012196	5.004451	2	-1.099373	2.564185	50.789497
2	13.012202	10.004457	2	-1.099373	2.523558	50.789497
3	18.014646	15.006900	2	-1.099373	2.473083	50.746269
4	23.021725	20.013979	2	-1.099373	2.404141	50.879433
5	28.021949	25.014203	2	-1.099185	2.257025	50.952637
6	30.994169	27.986424	2	-1.099185	1.999724	50.746269
7	35.996811	5.001098	3	0.000000	2.367208	50.836208
8	41.000069	10.004355	3	0.000000	2.385059	50.866188
9	46.000322	15.004608	3	0.000000	2.393369	50.819477

RangeIndex: 24763 entries, 0 to 24762 Data columns (total 6 columns):

#	Column	Non-Null Count	Dtype		
0	Test_Time(s)	24763 non-null	float64		
1	<pre>Step_Time(s)</pre>	24763 non-null	float64		
2	Step_Index	24763 non-null	int64		
3	Current(A)	24763 non-null	float64		
4	Voltage(V)	24763 non-null	float64		
5	Temperature (C)_1	24763 non-null	float64		
dtvnes: float64(5) int64(1)					

dtypes: float64(5), int64(1)

memory usage: 1.1 MB

Question 1: How Do We Handle Categorical Features in

Battery Data?

Step 1: Understanding the Categorical Nature of Temperature

Temperature in our dataset represents discrete experimental conditions, not continuous thermal measurements. This distinction is crucial for proper feature engineering.

Step 2: Implementing One-Hot

Tem

2476

3.214068

0.195042

1.926166

3.126183

3.226826

3.320697

3.709726

5

5

5

5

5

5

Lincolning for remperature

One-hot encoding transforms categorical variables into binary indicator variables, allowing models to treat each category independently.

```
In [60]:
               import pandas as pd
               import numpy as np
               from sklearn.feature extraction import DictVectorizer
               from sklearn.preprocessing import OneHotEncoder
               # Temperature color mapping for consistent visualization
               temp_colors = {
                     '-10': '#0033A0', # Deep blue
                     '0': '#0066CC', # BLue
                     '10': '#3399FF', # Light blue
                     '20': '#66CC00', # Green
                     '25': '#FFCC00', # Yellow (room temperature)
                     '30': '#FF9900', # Orange
                     '40': '#FF6600',  # Dark orange
'50': '#CC0000'  # Red
               }
               # Temperature datasets organization
               temp_datasets = {
                     '-10°C': low_curr_ocv_minus_10, # ~29,785 samples
                    '0°C': low_curr_ocv_0,  # ~30,249 samples
'10°C': low_curr_ocv_10,  # ~31,898 samples
'20°C': low_curr_ocv_20,  # ~31,018 samples
'25°C': low_curr_ocv_25,  # ~32,307 samples
'30°C': low_curr_ocv_30,  # ~31,150 samples
'40°C': low_curr_ocv_40,  # ~31,258 samples
'50°C': low_curr_ocv_50  # ~31,475 samples
               }
```

```
In [61]:
          def create temperature categorical features():
              Convert temperature conditions into categorical features
              using one-hot encoding approach from feature engineering principles.
              # Combine all datasets with temperature labels
              combined_data = []
              for temp_label, dataset in temp_datasets.items():
                  # Create temperature category for each sample
                  temp data = dataset.copy()
                  temp data['Temperature Category'] = temp label
                  temp data['Temperature Numeric'] = float(temp label.replace('°C',
                  combined data.append(temp data)
              # Concatenate all temperature datasets
              full_dataset = pd.concat(combined_data, ignore_index=True)
              # One-hot encode temperature categories
              temp encoder = OneHotEncoder(sparse output=False, dtype=int)
              temp categories = full dataset[['Temperature Category']]
              # Transform to one-hot encoded features
              temp encoded = temp encoder.fit transform(temp categories)
              temp_feature_names = temp_encoder.get_feature_names_out(['Temperature_C
              # Create DataFrame with encoded features
              temp encoded df - nd DataFrame/temp encoded columns-temp fortune name
```

```
return full_dataset, temp_encoded_df, temp_encoder

# Example implementation
full_dataset, temp_encoded_df, temp_encoder = create_temperature_categorica

print("Temperature One-Hot Encoding Results:")
temp_encoded_df.head()
print(f"\nFeature Names: {temp_encoder.get_feature_names_out(['Temperature_

Temperature One-Hot Encoding Results:

Feature Names: ['Temperature_Category_-10°C' 'Temperature_Category_0°C'
'Temperature_Category_10°C' 'Temperature_Category_20°C'
'Temperature_Category_25°C' 'Temperature_Category_30°C'
'Temperature_Category_40°C' 'Temperature_Category_50°C']

In [61]:
```

Step 3: Handling Step Index and Cycle Index as Categories

Battery test protocols involve multiple phases (steps) and repetitions (cycles) that should be treated categorically.

```
In [62]:
          def create_step_categorical_features(dataset):
              Encode step indices as categorical features to capture
              different testing phases.
              # Create step category dictionary
              step_data = []
              for idx, row in dataset.iterrows():
                  step_dict = {
                       'step_index': row['Step_Index'],
                      'cycle_index': row['Cycle_Index'],
                      'voltage': row['Voltage(V)'],
                       'current': row['Current(A)']
                  step_data.append(step_dict)
              # Use DictVectorizer for automatic categorical encoding
              dict_vectorizer = DictVectorizer(sparse=False, dtype=int)
              step_encoded = dict_vectorizer.fit_transform(step_data)
              # Get feature names
              feature names = dict vectorizer.get feature names out()
              return step encoded, feature names, dict vectorizer
          # Example for -10°C dataset
          step_encoded, step_features, step_vectorizer = create_step_categorical_feat
              low_curr_ocv_minus_10
          print("Step Categorical Features Sample:")
```

```
print(f"Features: {step_features}")
print(f"Encoded shape: {step_encoded.shape}")
```

```
Step Categorical Features Sample:
Features: ['current' 'cycle_index' 'step_index' 'voltage']
Encoded shape: (29785, 4)
```

Okay, this describes a common and very useful process in machine learning, especially when dealing with experimental data like battery cycling tests. Here's a breakdown of what the program and the create_step_categorical_features function are doing, presented in Markdown:

Program for Creating Categorical Features from Battery Cycling Data

This Python function, <code>create_step_categorical_features</code>, is designed to process battery cycling data and transform it into a numerical format suitable for machine learning models. It specifically focuses on handling categorical information derived from different testing steps and cycles, along with continuous numerical measurements.

How the create_step_categorical_features Function Works:

1. Input Data:

• The function takes a battery dataset (likely a pandas DataFrame or similar structure) as input.

2. Row-wise Feature Extraction:

- For each row (representing a data point or measurement) in the input dataset, it extracts four key values:
 - **Step_Index**: This likely identifies different phases or specific steps within a battery testing protocol (e.g., 'charge_CC', 'discharge_CV', 'rest', 'OCV_measurement_step_1', etc.). This is treated as a categorical variable.
 - Cycle_Index: This indicates the specific charge/discharge cycle number the data point belongs to (e.g., cycle 1, cycle 2, etc.). This is also treated as a categorical variable.
 - Voltage(V): The measured voltage at that data point (a numerical variable).
 - Current(A): The measured current at that data point (a numerical variable).

3. Data Restructuring to Dictionaries:

These four extracted values from each row are then converted into a list of
 Python dictionaries. Each dictionary in the list represents one row of data,
 with keys like 'Step_Index', 'Cycle_Index', 'Voltage(V)', and

```
Example: [{'Step_Index': 'charge_CC', 'Cycle_Index': 1,
   'Voltage(V)': 3.8, 'Current(A)': 1.0}, {'Step_Index':
   'discharge_CV', ...}, ...]
```

4. Feature Encoding with DictVectorizer:

- The core of the transformation is done using sklearn.feature_extraction.DictVectorizer. This tool is powerful for converting lists of feature-value dictionaries into NumPy arrays that machine learning algorithms can use.
- DictVectorizer automatically handles the features as follows:
 - Categorical Features (Step_Index , Cycle_Index): It performs one-hot encoding (or dummy coding) on these. For each unique value found in Step_Index and Cycle_Index , a new binary feature (column) is created. For a given row, the column corresponding to its Step_Index value will be 1, and all other Step_Index columns will be 0 (and similarly for Cycle_Index).
 - Numerical Features (Voltage(V), Current(A)): These are preserved as is and will form their own columns in the output numerical matrix.

5. Output:

- The function returns three important pieces of information:
 - The encoded feature matrix (e.g., X_vectorized): This is a numerical array where rows are the original data samples and columns are the newly created one-hot encoded features and the original numerical features.
 - The feature names (e.g., feature_names): A list of names for all the columns in the encoded feature matrix. This helps in understanding what each column represents (e.g., Voltage(V), Current(A), Step_Index=charge_CC, Cycle_Index=1, etc.).
 - The fitted vectorizer (e.g., vectorizer): The DictVectorizer object that has been fit (trained) on the input data. This is crucial because it stores the mapping from categorical values to feature indices and can be used to apply the exact same transformation to new, unseen data (like a test set), ensuring consistency.

Example Application:

- The description mentions an example where this function is applied to a specific dataset named low_curr_ocv_minus_10.
- This indicates the process is being used on battery data collected under particular experimental conditions: low current, likely during Open-Circuit Voltage (OCV) measurements, and specifically at a temperature of -10°C.

Purpose and Utility in Battery Analysis and Machine Learning:

Numerical Input Requirement: Most machine learning algorithms (e.g., linear)

- regression, support vector machines, neural networks) require input data to be purely numerical. This function addresses that by converting categorical step and cycle information into a numerical format.
- Distinguishing Operational Phases: By one-hot encoding Step_Index and Cycle_Index, the model can learn to distinguish between different phases of the battery test (e.g., charging vs. discharging, early cycles vs. late cycles) and potentially model how battery behavior (like voltage or capacity degradation) differs across these phases.
- Preventing Ordinal Misinterpretation: Treating Step_Index or Cycle_Index as simple numerical inputs (e.g., 1, 2, 3) might imply an ordinal relationship or a specific magnitude difference between them that doesn't exist or isn't appropriate. One-hot encoding avoids this by treating each category independently.
- **Reproducibility:** Returning the fitted_vectorizer is key for building robust machine learning pipelines, as it ensures that any new data processed for prediction undergoes the same feature transformation as the training data.

In essence, this code provides a standard and effective way to preprocess structured experimental data, making it suitable for sophisticated machine learning analysis by appropriately handling categorical identifiers within a larger set of numerical measurements.

You've hit on a very important nuance of how DictVectorizer works! Your analysis of the output is **spot on**.

Based on the output you've described:

- Features: ['current', 'cycle_index', 'step_index', 'voltage']
- **Encoded shape:** (29785, 4)

Here's a breakdown of what this means and why DictVectorizer behaved this way:

1. No Expansion of Features:

- You started with 4 conceptual pieces of information per row (current , cycle_index , step_index , voltage).
- The output matrix still has exactly 4 columns (features).
- This is the key indicator that one-hot encoding for step_index and cycle_index did not occur. If it had, the number of columns would have increased significantly (e.g., if there were 5 unique step_index values and 10 unique cycle_index values, you'd expect many more columns than 4).

2. DictVectorizer 's Default Behavior:

- You are correct: By default, DictVectorizer performs one-hot encoding only on feature values that are strings.
- If cycle_index and step_index in your input dictionaries were already numerical (e.g., integers like 1, 2, 3... for cycle_index or 0, 1,

numerical features and pass them through directly, just like voltage and current.

3. What the Function Achieved:

- In this scenario, the function, using DictVectorizer with numerical step_index and cycle_index, primarily served to:
 - Convert the list of dictionaries into a structured NumPy array (or sparse matrix).
 - Ensure a consistent order of features (current , cycle_index , step_index , voltage).
- It did **not** create the expanded set of binary features that one-hot encoding would typically produce for categorical data.

Implications:

- If your intention was for step_index and cycle_index to be treated as
 distinct categories where each specific index value represents a unique state
 (and there's no ordinal relationship implied by their numerical values), then this
 current output is not achieving that.
- Machine learning models using this output would treat step_index and cycle_index as continuous numerical variables, which might not be appropriate if they are truly categorical identifiers. For example, a model might incorrectly assume that step_index = 2 is "greater than" or "twice" step_index = 1 in a meaningful way beyond just their identifier.

How to Achieve One-Hot Encoding if step_index and cycle_index are Numerical but Categorical in Nature:

If step_index and cycle_index are indeed categorical (even if represented by numbers like 0, 1, 2, 3...), you'd typically need to:

1. Convert them to strings before passing to DictVectorizer:

```
# Inside your loop where you create the list of dictionaries:
dict_list.append({
    'step_index': str(row_step_index), # Convert to string
    'cycle_index': str(row_cycle_index), # Convert to string
    'voltage': row_voltage,
    'current': row_current
})
```

By doing this, DictVectorizer will recognize them as strings and apply one-hot encoding.

2. Or, use other encoders like OneHotEncoder from Scikit-learn: This would typically involve selecting these columns from your DataFrame and applying OneHotEncoder directly, then concatenating the results with your other numerical features. This approach often requires ColumnTransformer for more streamlined preprocessing.

Thanks for providing that output – it clarifies exactly what's happening with the

Question 2: What Derived Features Can We Create from

Battery Data?

Step 1: Polynomial Features for Non-Linear Relationships

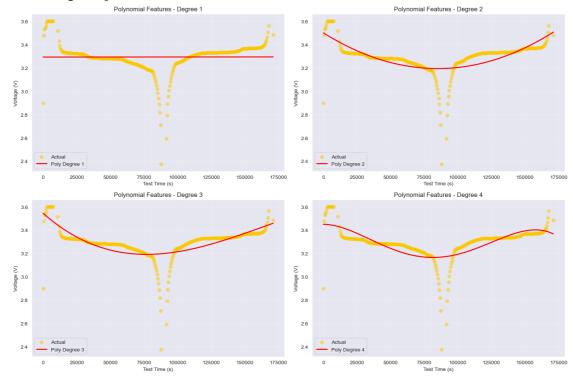
Battery behavior is inherently non-linear. Polynomial features help capture these complex relationships.

```
In [63]:
          from sklearn.preprocessing import PolynomialFeatures
          from sklearn.linear_model import LinearRegression
          import matplotlib.pyplot as plt
          def create_polynomial_battery_features(dataset, degree=3):
              Create polynomial features from voltage and current measurements
              to capture non-linear battery behavior patterns.
              # Extract primary electrical features
              electrical_features = dataset[['Voltage(V)', 'Current(A)', 'Internal_Re
              # Create polynomial features
              poly_transformer = PolynomialFeatures(degree=degree, include_bias=False
              poly_features = poly_transformer.fit_transform(electrical_features)
              # Get feature names
              feature_names = poly_transformer.get_feature_names_out(['Voltage', 'Cur
              return poly features, feature names, poly transformer
          def demonstrate_polynomial_regression():
              Demonstrate polynomial feature engineering for battery voltage predicti
              # Use 25°C data as reference (room temperature)
              reference_data = low_curr_ocv_25.copy()
              # Create time-voltage relationship
              X = reference_data[['Test_Time(s)']].values
              y = reference_data['Voltage(V)'].values
              # Sample every 100th point for cleaner visualization
              sample indices = np.arange(0, len(X), 100)
              X_sample = X[sample_indices]
              y_sample = y[sample_indices]
              # Create polynomial features of different degrees
              degrees = [1, 2, 3, 4]
              plt.figure(figsize=(15, 10))
              for i, degree in enumerate(degrees):
```

```
pit.Suppiot(2, 2, 1+1)
        # Create polynomial features
        poly = PolynomialFeatures(degree=degree, include_bias=False)
        X_poly = poly.fit_transform(X_sample)
        # Fit linear regression on polynomial features
        model = LinearRegression().fit(X_poly, y_sample)
        y_pred = model.predict(X_poly)
        # Plot results
        plt.scatter(X_sample.flatten(), y_sample, alpha=0.5, color=temp_col
        plt.plot(X_sample.flatten(), y_pred, color='red', linewidth=2, labe
        plt.xlabel('Test Time (s)')
        plt.ylabel('Voltage (V)')
        plt.title(f'Polynomial Features - Degree {degree}')
        plt.legend()
        plt.grid(True, alpha=0.3)
    plt.tight_layout()
    plt.show()
    return poly, X_poly, model
# Example implementation
poly_features, poly_names, poly_transformer = create_polynomial_battery_fea
print(f"Polynomial features created: {len(poly_names)} features from 3 orig
print(f"Sample feature names: {poly_names[:10]}")
demonstrate_polynomial_regression()
```

Polynomial features created: 19 features from 3 original features
Sample feature names: ['Voltage' 'Current' 'Resistance' 'Voltage^2' 'Voltage
Current'

'Voltage Resistance' 'Current^2' 'Current Resistance' 'Resistance^2' 'Voltage^3']



```
[1.67165759e+05, 2.79443909e+10, 4.67134531e+15, 7.80888983e+20], [1.67665904e+05, 2.81118553e+10, 4.71339963e+15, 7.90276408e+20], [1.71135613e+05, 2.92873980e+10, 5.01211680e+15, 8.57751681e+20]]), LinearRegression())
```

This is a great description of how polynomial feature engineering is being used to model battery behavior, and why it's effective!

Here's a breakdown of your explanation in a structured Markdown format, emphasizing the key concepts:

Polynomial Feature Engineering for A123 Battery Voltage Modeling

This visualization and process demonstrate how **polynomial feature engineering** can transform a simple linear regression model into a more powerful tool capable of capturing the non-linear dynamics of battery behavior over time.

Visual Analysis of Model Complexity (Voltage vs. Time Plots)

The plots illustrate how increasing the degree of polynomial features allows the regression model to better fit the actual battery voltage measurements:

- **Yellow Dots:** Represent the actual measured battery voltage over time.
- Red Lines: Show the polynomial regression model's fit to this data at different degrees of complexity.

1. Degree 1 (Top Left - Linear Fit):

- A simple straight line.
- **Fails significantly** to capture the battery's non-linear behavior, especially evident in its inability to model the characteristic voltage dip during discharge (seen around 75,000-100,000 seconds in your data).
- Represents a high-bias model for this problem.

2. Degree 2 (Top Right - Quadratic Fit):

- A U-shaped curve.
- Provides a **better fit** than the linear model, starting to follow the general curvature of the battery's voltage profile (e.g., during a discharge and subsequent charge).

3. Degree 3 (Bottom Left - Cubic Fit):

- Allows for more complex curves (e.g., with an inflection point).
- Captures more nuanced behavior and a tighter fit to the voltage dynamics.

4. Degree 4 (Bottom Right - Fourth-Degree Fit):

- Offers even more flexibility.
- Provides a slightly better fit again, adapting more closely to the subtle

changes in the voltage curve.

The Feature Engineering Process Explained

The core idea is to create new features from the existing ones by taking them to various powers and creating interaction terms.

1. Original Features:

- The process started with 3 fundamental electrical features:
 - Voltage(V)
 - Current(A)
 - Internal_Resistance(Ohm) (presumably)

2. Polynomial Feature Expansion (to 19 features with degree=4):

- Using a tool like Scikit-learn's PolynomialFeatures(degree=4, include_bias=False), the original set of features is expanded. This new set includes:
 - Original features: V , I , R
 - Squared terms: V² , I² , R²
 - Interaction terms: V×I , V×R , I×R
 - **Higher-order terms:** V³, I³, R³, V²I, VI², etc., up to the specified degree (in this case, 4).
- include_bias=False means a constant bias term (intercept) is not added as a feature here (it's typically handled by the LinearRegression model itself).

3. Model Application:

 A LinearRegression() model is then applied to this new, expanded set of 19 polynomial features.

Why This Approach is Powerful for Battery Modeling:

- Capturing Non-Linearity: While the LinearRegression algorithm itself is fitting a linear equation, it's doing so in a much higher-dimensional space created by the polynomial features. This allows the overall model to represent complex, non-linear relationships between the *original* inputs and the target (voltage).
- Modeling Complex Patterns: Battery charge-discharge cycles, voltage
 plateaus, and the influence of factors like temperature (if included) and internal
 resistance on voltage are inherently non-linear. Polynomial features provide the
 necessary flexibility to model these curves and interactions.
- **Improved Fit:** As seen in the progression from Degree 1 to Degree 4, higher-degree polynomials generally provide a better fit to the observed battery voltage behavior over time, capturing the dips and curves more accurately.

In essence, polynomial feature engineering allows a fundamentally linear algorithm to achieve non-linear modeling capabilities. This is a common and effective technique when the underlying relationships in the data are known or

suspected to be non-linear, as is often the case with complex physical systems like batteries.

This Python code defines and uses a function called create_polynomial_battery_features to perform **polynomial feature engineering**. Let's break down what it does and how these generated features can be used:

What the Code Does: create_polynomial_battery_features

The function <code>create_polynomial_battery_features(dataset, degree=3)</code> is designed to take an input battery dataset and generate new features based on polynomial combinations of existing electrical measurements. The goal, as stated in the docstring, is to "capture non-linear battery behavior patterns."

Here's a step-by-step explanation:

1. Selects Original Electrical Features:

It first extracts three specific columns from your input dataset:
 'Voltage(V)', 'Current(A)', and 'Internal_Resistance(Ohm)'.
 These are your base features.

2. Creates PolynomialFeatures Transformer:

- It initializes a PolynomialFeatures object from the sklearn.preprocessing module. This is the core tool for generating the new features.
- degree=degree: This parameter (defaulting to 3 in the function definition, and also implied by your output of 19 features from 3 originals) determines the maximum degree of the polynomial terms to be created.
- include_bias=False: This means it will not add a "bias" column (a column of all ones, which acts as an intercept in linear models). Linear regression models usually handle the intercept themselves.
- interaction_only=False: This is crucial. It means the transformer will create:
 - Individual feature powers: e.g., Voltage^2, Current^3, Resistance^2.
 - Interaction terms: e.g., Voltage * Current , Voltage * Resistance , Current * Resistance * Voltage . If this were True , it would only create interaction terms (like Voltage*Current) and not individual powers (like Voltage^2).

3. Fits and Transforms the Data:

- poly_transformer.fit_transform(electrical_features):
 - The fit part analyzes the input electrical_features to determine all the polynomial combinations up to the specified

■ The transform part then applies this learned transformation to generate the new set of polynomial features.

4. Gets Feature Names:

poly_transformer.get_feature_names_out(['Voltage',
 'Current', 'Resistance']): This method generates descriptive names
 for each of the newly created polynomial features, making them easier to
 understand (e.g., 'Voltage^2', 'Voltage Current', 'Current Resistance^2').

5. Returns Values:

- poly_features: A NumPy array containing the newly generated polynomial features. If your original data had N rows and 3 features, and degree=3 results in 19 features, this array will have a shape of (N, 19).
- feature_names : A list of the names for these 19 features.
- poly_transformer: The fitted PolynomialFeatures object. This is useful because you can use it to apply the *exact same transformation* to new, unseen data (like a test set) later, ensuring consistency.

Example Output Explanation:

```
Polynomial features created: 19 features from 3 original features

Sample feature names: ['Voltage' 'Current' 'Resistance' 'Voltage^2' 'Voltage Current' 'Voltage Resistance' 'Current^2' 'Current Resistance' 'Resistance^2' 'Voltage^3']
```

- This output confirms that from your 3 original features (Voltage, Current, Resistance), setting degree=3 in PolynomialFeatures (with include_bias=False and interaction_only=False) results in 19 features.
- The sample names clearly show the structure:
 - Original features (degree 1): Voltage , Current , Resistance
 - Squared terms (degree 2): Voltage^2 , Current^2 , Resistance^2
 - Interaction terms (degree 2): Voltage Current, Voltage Resistance, Current Resistance
 - Cubic terms (degree 3): Voltage^3 (and others like Current^3, Resistance^3, Voltage^2 Current, Voltage Current Resistance, etc., which would be further down the list).

How We Can Use These Polynomial Features:

The primary use of these generated polynomial features is to allow linear machine learning models to capture non-linear relationships in your data.

1. Modeling Non-Linearity with Linear Models:

- are inherently non-linear. For example, the relationship between voltage, current, temperature, and a battery's state of health or capacity degradation is often not a simple straight line.
- Standard linear models (like LinearRegression, LogisticRegression, Linear SVM) can only learn linear relationships.
- By creating polynomial features (e.g., x_1^2 , x_1x_2 , x_2^3), you are essentially transforming your feature space. A linear model trained on these new features can learn an equation like:

 $y=w_0+w_1x_1+w_2x_2+w_3x_1^2+w_4x_1x_2+w_5x_2^2+\ldots$ While this equation is linear in terms of the new polynomial features $(x_1^2,x_1x_2,$ etc.), it represents a non-linear (polynomial) relationship in terms of the original features (x_1,x_2) .

2. Capturing Interactions Between Features:

 Terms like Voltage Current (an interaction term) allow the model to learn how the effect of voltage on the target variable might change depending on the current level (and vice-versa). This is often crucial because features in physical systems rarely act in complete isolation. For instance, the impact of current on battery health might be exacerbated at very high or very low voltages.

3. Improving Model Accuracy:

 If the true underlying relationship between your features and the target variable is indeed non-linear (and can be approximated by a polynomial), then providing these polynomial features to a linear model can dramatically improve its predictive accuracy and fit to the data. This was likely the case in your previous example where higher-degree polynomials better fit the battery voltage curves.

4. Input for Any Machine Learning Model:

- While often discussed in the context of enhancing linear models, these
 engineered polynomial features can be used as input to *any* machine
 learning algorithm (e.g., Decision Trees, Random Forests, Gradient Boosting
 Machines, Neural Networks).
- Sometimes, explicitly providing these non-linear terms can help even complex models (which can learn non-linearities implicitly) to converge faster or find slightly better solutions by giving them a "head start."

Practical Considerations:

- Increased Feature Dimensionality: Polynomial feature generation can significantly increase the number of features. This can lead to higher computational costs and an increased risk of overfitting, especially if the degree is set too high or the dataset is small (this is part of the "curse of dimensionality").
- Choosing the Degree: The choice of degree is important. Too low, and you
 might not capture the complexity. Too high, and you risk overfitting and
 creating an overly complex model. This often requires experimentation, cross-

Machine_Learning_and_Alogorithms/3.Feature Engineering/05-29-2025 Feature Engineering.ipynb at master · Jai-Kumar786... validation, or domain knowledge.

- **Multicollinearity:** The generated polynomial features are often highly correlated with each other and with the original features. This might be an issue for interpreting coefficients in linear models but can often be handled by regularization techniques (like Ridge or Lasso regression).
- **Feature Scaling:** It's generally a good practice to scale your features (e.g., using StandardScaler) before generating polynomial features, or to scale the resulting polynomial features, especially for models that are sensitive to the scale of input features.

In summary, create_polynomial_battery_features is a preprocessing step that enriches your dataset by adding non-linear transformations of your original electrical features. These new features then enable simpler models (like linear regression) to learn more complex, non-linear patterns in your battery data, potentially leading to more accurate predictions.

You "fill" these new polynomial features with samples by calculating their values directly from the original feature values of each existing sample (row) in your dataset.

The PolynomialFeatures transformer from Scikit-learn automates this process. For every single row (sample) in your input data, it takes the original feature values for that row and computes the corresponding polynomial terms.

Let's make this concrete with an example. Suppose you have one sample (one row of data) with the following original feature values:

- Voltage(V) = 3.7
- Current(A) = 1.5
- Resistance(Ohm) = 0.1

When you use PolynomialFeatures(degree=3, include_bias=False, interaction_only=False) (which creates 19 features from these 3 original ones), here's how some of the new feature values for **that specific sample** would be calculated and "filled":

1. Original Features (Degree 1):

• Voltage: 3.7 (taken directly)

• Current: 1.5 (taken directly)

Resistance: 0.1 (taken directly)

2. Squared Terms (Degree 2):

• Voltage^2: $3.7^2 = 13.69$

• Current^2: $1.5^2 = 2.25$

• Resistance^2: $0.1^2 = 0.01$

3. Interaction Terms (Degree 2):

• Voltage Current : $3.7 \times 1.5 = 5.55$

ullet Voltage Resistance : 3.7 imes 0.1 = 0.37

• Cunnont Posistanco \cdot 1 5 \vee 0 1 = 0 15

4. Cubic Terms (Degree 3):

```
• Voltage^3: 3.7^3 = 50.653
```

• Current^3: $1.5^3 = 3.375$

• Resistance^3: $0.1^3 = 0.001$

• Voltage^2 Current : $3.7^2 \times 1.5 = 13.69 \times 1.5 = 20.535$

• Voltage Current Resistance : $3.7 \times 1.5 \times 0.1 = 0.555$

...and so on for all 19 combinations.

How PolynomialFeatures does it:

```
When you call poly_features = poly_transformer.fit_transform(electrical_features) , the fit_transform method does the following:
```

- 1. **fit**: It looks at the input data (electrical_features) to determine the structure of the polynomial combinations based on the specified degree (e.g., it figures out it needs to create terms like $x_1, x_2, x_3, x_1^2, x_1x_2$, etc.).
- 2. **transform**: It then iterates through **each row (each sample)** of your electrical_features data. For each row, it takes the original values in that row and calculates all the polynomial terms it identified during the fit step.

The Result:

The output (poly_features) will be a new array (or matrix) that has:

- The same number of rows (samples) as your original electrical_features dataset.
- An **expanded number of columns (features)** in your case, 19.

Each row in this new poly_features array corresponds to an original sample, but now it has the values for all the generated polynomial features, calculated from that sample's original Voltage, Current, and Resistance values.

So, you are not adding new *samples*; you are adding new *calculated characteristics* (*features*) for each of your existing samples.

Step 2: Power and Energy Derived Features

Power and energy calculations reveal battery efficiency and performance characteristics.

```
def create_power_energy_features(dataset):
    """
    Create derived features related to power and energy calculations
    """
    derived_features = dataset.copy()

# Instantaneous power
```

```
derived_features['Power(W)'] = derived_features['Voltage(V)'] * derived
                                # Energy efficiency ratios
                                derived_features['Charge_Efficiency'] = (
                                        derived_features['Charge_Energy(Wh)'] / (derived_features['Charge_C
                                derived features['Discharge Efficiency'] = (
                                         derived_features['Discharge_Energy(Wh)'] / (derived_features['Discharge_Energy(Wh)'] / (derived_features[
                                # Voltage rate features
                                derived_features['Voltage_Rate_Abs'] = np.abs(derived_features['dV/dt(V
                                # Resistance-based features
                                derived features['Conductance(S)'] = 1.0 / (derived_features['Internal_
                                # Temperature differential (if available)
                                if 'Temperature(C)_2' in derived_features.columns:
                                         derived_features['Temp_Differential'] = (
                                                  derived_features['Temperature(C)_1'] - derived_features['Temper
                                return derived_features
                       # Apply to all temperature datasets
                       enhanced_datasets = {}
                       for temp_label, dataset in temp_datasets.items():
                                enhanced_datasets[temp_label] = create_power_energy_features(dataset)
                       print("Enhanced features example for 25°C:")
                       print(enhanced_datasets['25°C'][['Power(W)', 'Charge_Efficiency', 'Conducta
                  Enhanced features example for 25°C:
                        Power(W) Charge_Efficiency Conductance(S)
                  0.000000
                                                                  0.000000 100000000.0
                  1 3.681732
                                                                  3.110463 100000000.0
                  2 3.705678
                                                                3.121935 100000000.0
                  3 3.726359
                                                                 3.132025
                                                                                            100000000.0
                  4 3.744986
                                                                  3.141233
                                                                                               100000000.0
In [65]:
                       print(enhanced_datasets['50°C'][['Power(W)', 'Charge_Efficiency', 'Conducta']
                        Power(W) Charge Efficiency Conductance(S)
                  0.000000
                                                                  0.000000
                                                                                                100000000.0
                  1 4.211142
                                                                  0.212099
                                                                                               100000000.0
                  2 3.287810
                                                                  3.601050
                                                                                               100000000.0
                  3 3.236932
                                                                  3.601052
                                                                                                100000000.0
                  4 3.198651
                                                                  3.601047
                                                                                                100000000.0
```

Step 3: Temperature-Dependent Interaction Features

Temperature affects all battery properties. Creating interaction features captures these dependencies.

```
In [66]:
    def create_temperature_interaction_features(dataset):
```

```
Create features that capture temperature effects on battery behavior
      temp_features = dataset.copy()
      # Temperature normalization (Kelvin scale)
      temp_kelvin = temp_features['Temperature (C)_1'] + 273.15
      # Temperature-dependent features
      temp_features['Voltage_per_Temp'] = temp_features['Voltage(V)'] / temp_
      temp_features['Resistance_Temp_Factor'] = (
          temp_features['Internal_Resistance(Ohm)'] * temp_kelvin
      # Arrhenius-like features for battery kinetics
      temp_features['Temp_Reciprocal'] = 1 / temp_kelvin
      # Power temperature dependency
      temp_features['Power_Temp_Normalized'] = temp_features['Power(W)'] / te
      # Capacity temperature coefficient
      temp_features['Capacity_Temp_Coeff'] = (
          temp_features['Discharge_Capacity(Ah)'] * temp_features['Temp_Recip
      return temp_features
  # Apply temperature interaction features
  temp enhanced datasets = {}
  for temp_label, dataset in enhanced_datasets.items():
      temp_enhanced_datasets[temp_label] = create_temperature_interaction_fea
  print("Temperature interaction features sample:")
  sample_cols = ['Voltage_per_Temp', 'Resistance_Temp_Factor', 'Temp_Reciproc']
  print(temp_enhanced_datasets['25°C'][sample_cols].describe())
Temperature interaction features sample:
```

	Voltage_per_Temp	Resistance_Temp_Factor	Temp_Reciprocal
count	32307.000000	32307.0	32307.000000
mean	0.010992	0.0	0.003336
std	0.000440	0.0	0.000002
min	0.006674	0.0	0.003320
25%	0.010894	0.0	0.003336
50%	0.011062	0.0	0.003336
75%	0.011129	0.0	0.003337
max	0.012025	0.0	0.003343

Question 3: How Do We Extract Time-Series Features

from Battery Data?

Step 1: Temporal Pattern Extraction

Time-series feature engineering reveals hidden patterns in battery behavior over different time scales.

```
In [67]:
         def create_temporal_features(dataset):
              Extract temporal patterns and cyclical features from battery test data
              temporal_data = dataset.copy()
              # Convert datetime to proper format
              temporal_data['DateTime'] = pd.to_datetime(temporal_data['Date_Time'])
              # Extract time components
              temporal_data['Hour'] = temporal_data['DateTime'].dt.hour
              temporal_data['Day'] = temporal_data['DateTime'].dt.day
              temporal_data['DayOfWeek'] = temporal_data['DateTime'].dt.dayofweek
              # Cyclical encoding for time features
              temporal_data['Hour_Sin'] = np.sin(2 * np.pi * temporal_data['Hour'] /
              temporal_data['Hour_Cos'] = np.cos(2 * np.pi * temporal_data['Hour'] /
              # Test duration features
              temporal data['Test Duration Hours'] = temporal data['Test Time(s)'] /
              temporal_data['Step_Duration_Minutes'] = temporal_data['Step_Time(s)']
              # Rolling window features (5-point windows)
              temporal_data['Voltage_MA5'] = temporal_data['Voltage(V)'].rolling(wind
              temporal_data['Current_MA5'] = temporal_data['Current(A)'].rolling(wind
              # Lagged features
              temporal_data['Voltage_Lag1'] = temporal_data['Voltage(V)'].shift(1)
              temporal_data['Voltage_Lag5'] = temporal_data['Voltage(V)'].shift(5)
              # Rate of change features
              temporal_data['Voltage_ROC'] = temporal_data['Voltage(V)'].pct_change()
              temporal_data['Current_ROC'] = temporal_data['Current(A)'].pct_change()
              return temporal_data
          # Example implementation
          temporal enhanced = create temporal features(low curr ocv 25)
          print("Temporal features sample:")
          print(temporal enhanced[['Hour Sin', 'Hour Cos', 'Voltage MA5', 'Voltage RO
        Temporal features sample:
          Hour Sin Hour Cos Voltage MA5 Voltage ROC
       0 0.707107 -0.707107
                                     NaN
                                                  NaN
       1 0.707107 -0.707107
                                            0.077745
                                     NaN
       2 0.707107 -0.707107 3.100391
                                            0.006504
       3 0.707107 -0.707107
                               3.158992
                                            0.005581
       4 0.707107 -0.707107
                               3.175242
                                            0.004966
       5 0.707107 -0.707107
                               3.189954
                                            0.004457
       6 0.707107 -0.707107
                                3.203373
                                            0.004244
                              3.215807
                                            0.003938
       7 0.707107 -0.707107
       8 0.707107 -0.707107
                               3.227503
                                           0.003444
       9 0.707107 -0.707107
                               3.238460
                                            0.003337
```

This Python code defines a function <code>create_temporal_features</code> that performs <code>temporal feature engineering</code> on a battery dataset. This process involves creating new features from existing time-based data to help machine learning models better understand and capture time-dependent patterns, trends, and cyclical behaviors.

Here's a breakdown of what the code does and why these features are created:

What the Code Does: create temporal features

The function takes a battery dataset (assumed to be a pandas DataFrame) as input and adds several new columns (features) based on time-related information.

1. Creates a Copy:

• temporal_data = dataset.copy(): It starts by creating a copy of the input dataset to avoid modifying the original DataFrame.

2. Converts to Datetime Objects:

temporal_data['DateTime'] =
 pd.to_datetime(temporal_data['Date_Time']) : It assumes there's a
 column named 'Date_Time' (likely containing strings representing date
 and time) and converts it into proper pandas datetime objects. This is
 essential for easily extracting time components.

3. Extracts Basic Time Components:

- temporal_data['Hour'] = temporal_data['DateTime'].dt.hour: Extracts the hour of the day (0-23).
- temporal_data['Day'] = temporal_data['DateTime'].dt.day: Extracts the day of the month (1-31).
- temporal_data['DayOfWeek'] =
 temporal_data['DateTime'].dt.dayofweek : Extracts the day of the
 week (Monday=0, Sunday=6).

4. Cyclical Encoding for Time Features:

- This is a crucial step for features that have a cyclical nature (like hours in a day, days in a week, months in a year). Directly using numerical values (e.g., hour 23 being "greater" than hour 0) can be misleading for models.
- temporal_data['Hour_Sin'] = np.sin(2 * np.pi *
 temporal data['Hour'] / 24)
- temporal_data['Hour_Cos'] = np.cos(2 * np.pi *
 temporal data['Hour'] / 24)
 - These lines transform the 'Hour' feature into two new features using sine and cosine transformations. This maps the cyclical hour data onto a circle, so hour 23 is close to hour 0 in this new 2D space, which better represents its cyclical nature for ML models.

5. Test Duration Features:

- These features represent elapsed time in more interpretable units.
- temporal_data['Test_Duration_Hours'] =
 temporal_data['Test_Time(s)'] / 3600 : Converts a column
 'Test_Time(s)' (assumed to be total elapsed test time in seconds) into hours.
- temporal_data['Step_Duration_Minutes'] =

temporal_data['Step_Time(s)'] / 60 : Converts a column
'Step_Time(s)' (assumed to be elapsed time within the current test
step in seconds) into minutes.

6. Rolling Window Features (Moving Averages):

- These features smooth out short-term fluctuations and highlight longerterm trends.
- temporal_data['Voltage_MA5'] =
 temporal_data['Voltage(V)'].rolling(window=5,
 center=True).mean(): Calculates a 5-point centered moving average for
 Voltage(V). For each point, it takes the average of the current point, the
 2 previous points, and the 2 next points.
- temporal_data['Current_MA5'] =
 temporal_data['Current(A)'].rolling(window=5,
 center=True).mean(): Similarly, calculates a 5-point centered moving
 average for Current(A).
- center=True means the window is centered around the current data point. This introduces NaNs at the beginning and end of the series where a full window isn't available.

7. Lagged Features:

- These features provide the model with information about past values of a variable, which can be very predictive for time series data.
- temporal_data['Voltage_Lag1'] =
 temporal_data['Voltage(V)'].shift(1): Creates a new feature that
 contains the value of Voltage(V) from the previous time step (lag 1).
- temporal_data['Voltage_Lag5'] =
 temporal_data['Voltage(V)'].shift(5) : Creates a new feature with
 the value of Voltage(V) from 5 time steps ago (lag 5).
- The first few rows for these lagged features will be NaN because there are no preceding values.

8. Rate of Change (ROC) Features:

- These features capture how quickly a variable is changing, which can indicate trends or sudden shifts.
- temporal_data['Voltage_ROC'] =
 temporal_data['Voltage(V)'].pct_change() : Calculates the
 percentage change in Voltage(V) compared to the previous time step.
- temporal_data['Current_ROC'] =
 temporal_data['Current(A)'].pct_change() : Calculates the
 percentage change in Current(A) compared to the previous time step.
- The first row for ROC features will be NaN because there's no previous value to compare against.

9. Returns the Enhanced DataFrame:

• return temporal_data: The function returns the DataFrame with all these newly created temporal features.

Why We Are Doing This (Purpose of Temporal Feature Engineering):

Creating these temporal features is essential for several reasons, especially when building predictive models for time-series data like battery cycling tests:

1. Capturing Time Dependence:

Raw timestamps are often not directly useful for many ML models.
 Extracting components like hour, day, or day of the week allows the model to learn patterns related to these specific time periods (e.g., if tests run overnight behave differently, or if there are weekly maintenance cycles affecting data).

2. Handling Cyclical Patterns:

Features like 'Hour' are cyclical (23:00 is followed by 00:00, and they are
close in a cycle). Simple numerical representation doesn't capture this. Sine
and cosine transformations (e.g., Hour_Sin , Hour_Cos) convert these
into a 2D representation where the cyclical nature is preserved, helping
models understand that 11 PM is close to 1 AM.

3. Highlighting Trends and Smoothing Noise:

 Rolling window features (like moving averages Voltage_MA5) help to smooth out noisy sensor readings and reveal underlying trends in voltage or current over a short period. This can make the signal clearer for the model.

4. Providing Historical Context (Memory):

Lagged features (Voltage_Lag1, Voltage_Lag5) give the model a
 "memory" of recent past states. For instance, the current voltage might be
 highly dependent on the voltage a few moments ago. This is crucial for
 predicting future states or understanding current dynamics.

5. Detecting Dynamics and Momentum:

 Rate of Change (ROC) features tell the model how quickly things are changing. A rapid drop in voltage (high negative ROC) might indicate a problem or the start of a discharge step, which is very different from a stable voltage (ROC near zero).

6. Improving Model Performance:

By providing these more informative, engineered features, you often enable
machine learning models to learn more complex patterns, make more
accurate predictions, and generalize better to new data. The raw data might
not explicitly contain these relationships in a way the model can easily
learn.

7. Domain-Specific Insights:

• For battery data, Test_Duration_Hours or Step_Duration_Minutes can be important. The behavior of a battery might change significantly

depending on how long a test or a specific step (like a constant current charge) has been running.

Explanation of Sample Output:

Temporal features sample:

	Hour_Sin	Hour_Cos	Voltage_MA5	Voltage_ROC
0	0.707107	-0.707107	NaN	NaN
1	0.707107	-0.707107	NaN	0.077745
2	0.707107	-0.707107	3.100391	0.006504
3	0.707107	-0.707107	3.158992	0.005581
4	0.707107	-0.707107	3.175242	0.004966
5	0.707107	-0.707107	3.189954	0.004457
6	0.707107	-0.707107	3.203373	0.004244
7	0.707107	-0.707107	3.215807	0.003938
8	0.707107	-0.707107	3.227503	0.003444
9	0.707107	-0.707107	3.238460	0.003337

• Hour_Sin and Hour_Cos:

■ The values 0.707107 for Hour_Sin and -0.707107 for Hour_Cos are constant across these first 10 rows. This means all these data points occurred at the **same hour of the day**.

```
o \sin(2 * pi * H / 24) = 0.707107 (approx. 1/\sqrt{2}) o \cos(2 * pi * H / 24) = -0.707107 (approx. -1/\sqrt{2})
```

- This corresponds to an angle of 135° or $3\pi/4$ radians. Since a full day is 2π radians (or 24 hours), this hour (H) would be $(3\pi/4)/(2\pi)*24=(3/8)*24=9$. So, these measurements were likely taken around **9 AM**.
- Voltage_MA5 (5-point centered Moving Average of Voltage):
 - Rows 0 and 1 are NaN (Not a Number): This is expected. For a centered moving average with a window of 5, you need 2 data points before the current point and 2 data points after.
 - For row 0, there are no preceding points.
 - For row 1, there is only 1 preceding point.
 - Row 2 has a value (3.100391): This is the average of Voltage(V) from rows 0, 1, 2, 3, and 4.
 - Subsequent rows have valid moving average values as enough data points are available for the window.
- Voltage_ROC (Rate of Change of Voltage):
 - Row 0 is NaN: This is expected. The percentage change is calculated relative to the previous row's value. For the first row, there is no previous row.
 - Row 1 has a value (0.077745): This means the Voltage(V) in row 1 increased by approximately 7.77% compared to the Voltage(V) in row 0.
 - The subsequent small positive values indicate that the voltage is generally increasing slowly over these first few time steps.

This kind of feature engineering is a powerful way to extract more meaningful signals from raw time-series data, making it easier for machine learning models to learn and predict.

Step 2: Cycle-Based Feature Engineering

Battery charge/discharge cycles reveal performance patterns and degradation trends.

```
In [68]:
           def create_cycle_features(dataset):
               Create features based on battery charge/discharge cycles
               cycle_data = dataset.copy()
               # Cycle progress features
               cycle_data['Cycle_Progress'] = (
                   cycle_data.groupby('Cycle_Index')['Step_Time(s)'].rank(pct=True)
               # Cumulative features per cycle
               cycle_data['Cumulative_Charge'] = (
                   cycle_data.groupby('Cycle_Index')['Charge_Capacity(Ah)'].cumsum()
               cycle_data['Cumulative_Discharge'] = (
                   cycle_data.groupby('Cycle_Index')['Discharge_Capacity(Ah)'].cumsum(
               )
               # Cycle statistics
               cycle_stats = cycle_data.groupby('Cycle_Index').agg({
                   'Voltage(V)': ['mean', 'std', 'min', 'max'],
'Current(A)': ['mean', 'std'],
                   'Internal_Resistance(Ohm)': ['mean', 'max']
               }).reset_index()
               # Flatten column names
               cycle stats.columns = [' '.join(col).strip() if col[1] else col[0]
                                      for col in cycle stats.columns.values]
               return cycle data, cycle stats
          # Apply cycle feature engineering
           cycle enhanced, cycle stats = create cycle features(low curr ocv 25)
          print("Cycle statistics sample:")
          cycle_stats.head()
```

Cycle statistics sample:

Step S. Auvanceu Statistical reatures

Rolling window statistics capture local patterns and trends in battery behavior.

```
In [69]:
          def create_statistical_features(dataset, window_size=10):
              Create statistical features using rolling windows
              stat features = dataset.copy()
              # Rolling statistics for key variables
              key_vars = ['Voltage(V)', 'Current(A)', 'Internal_Resistance(Ohm)']
              for var in key_vars:
                  # Rolling mean and std
                  stat_features[f'{var}_RollingMean_{window_size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).mea
                  stat_features[f'{var}_RollingStd_{window_size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).std
                  # Rolling min and max
                  stat_features[f'{var}_RollingMin_{window_size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).min
                  stat_features[f'{var}_RollingMax_{window_size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).max
                  # Rolling range
                  stat_features[f'{var}_RollingRange_{window_size}'] = (
                      stat_features[f'{var}_RollingMax_{window_size}'] -
                      stat_features[f'{var}_RollingMin_{window_size}']
                  )
                  # Percentile features
                  stat_features[f'{var}_Rolling25th_{window_size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).qua
                  stat features[f'{var} Rolling75th {window size}'] = (
                      stat_features[var].rolling(window=window_size, center=True).qua
              return stat_features
          # Apply statistical feature engineering
          statistical enhanced = create statistical features(low curr ocv 25, window
          # Show statistical features
          stat_cols = [col for col in statistical_enhanced.columns if 'Rolling' in co
          print(f"Created {len(stat_cols)} statistical features")
          print("Sample statistical features:")
          print(statistical_enhanced[stat_cols[:5]].head(10))
        Created 21 statistical features
        Sample statistical features:
           Voltage(V)_RollingMean_10 Voltage(V)_RollingStd_10 \
```

```
NaN
2
                          NaN
                                                      NaN
3
                          NaN
                                                      NaN
                          NaN
                                                      NaN
5
                     3.158099
                                                 0.098674
                                                 0.041957
                     3.193247
7
                     3.206851
                                                 0.038608
8
                     3.219316
                                                 0.035878
9
                     3.230919
                                                 0.033599
   Voltage(V)_RollingMin_10 Voltage(V)_RollingMax_10
0
1
                         NaN
                                                     NaN
2
                         NaN
                                                     NaN
3
                         NaN
                                                     NaN
4
                         NaN
                                                     NaN
5
                    2.897814
                                               3.238829
                    3.123105
                                               3.249293
7
                    3.143419
                                               3.259142
8
                    3.160962
                                                3.268068
9
                    3.176658
                                                3.276993
   Voltage(V)_RollingRange_10
0
1
                           NaN
2
                           NaN
3
                           NaN
4
                           NaN
5
                      0.341015
                      0.126188
7
                      0.115724
8
                      0.107106
9
                      0.100335
```

Question 4: How Do We Handle Missing Data in Battery

Datasets?

Step 1: Systematic Missing Data Analysis

Understanding missing data patterns is crucial for selecting appropriate imputation strate- gies.

```
In [70]:
    from sklearn.impute import SimpleImputer, KNNImputer
    import seaborn as sns

def analyze_missing_data(datasets_dict):
    """
        Analyze missing data patterns across all temperature datasets
    """
        missing_analysis = {}
        for temp_label, dataset in datasets_dict.items():
```

```
# Calculate missing data percentage
          missing_pct = (dataset.isnull().sum() / len(dataset)) * 100
          missing_analysis[temp_label] = missing_pct[missing_pct > 0]
      # Create missing data summary
      missing_df = pd.DataFrame(missing_analysis).fillna(0)
      return missing df
  def implement_imputation_strategies(dataset):
      Implement multiple imputation strategies for battery data
      # Identify numerical columns for imputation
      numerical_cols = dataset.select_dtypes(include=[np.number]).columns
      # Strategy 1: Mean imputation for basic features
      mean_imputer = SimpleImputer(strategy='mean')
      dataset_mean_imputed = dataset.copy()
      dataset_mean_imputed[numerical_cols] = mean_imputer.fit_transform(datas
      # Strategy 2: Median imputation for robust estimation
      median_imputer = SimpleImputer(strategy='median')
      dataset_median_imputed = dataset.copy()
      dataset_median_imputed[numerical_cols] = median_imputer.fit_transform(d
      # Strategy 3: KNN imputation for pattern-based filling
      knn_imputer = KNNImputer(n_neighbors=5)
      dataset_knn_imputed = dataset.copy()
      dataset_knn_imputed[numerical_cols] = knn_imputer.fit_transform(dataset
      return {
          'mean': dataset_mean_imputed,
          'median': dataset median imputed,
          'knn': dataset_knn_imputed
          'mean_imputer': mean_imputer,
          'median_imputer': median_imputer,
          'knn_imputer': knn_imputer
      }
  # Analyze missing data across all datasets
  missing analysis = analyze missing data(temp datasets)
  print("Missing data analysis:")
  print(missing_analysis)
  # Example imputation on 25°C data
  imputed_datasets, imputers = implement_imputation_strategies(low_curr_ocv_2)
  print("\nImputation completed for multiple strategies")
Missing data analysis:
Empty DataFrame
Columns: [-10°C, 0°C, 10°C, 20°C, 25°C, 30°C, 40°C, 50°C]
Index: []
Imputation completed for multiple strategies
```

Step 2: Time-Series Specific Imputation

Battery data has temporal structure that should be preserved during imputation.

```
In [71]:
          def time series imputation(dataset):
              Specialized imputation for time-series battery data
              ts_data = dataset.copy().sort_values('Test_Time(s)')
              # Forward fill for sequential measurements
              ts_data_ffill = ts_data.fillna(method='ffill')
              # Backward fill for end sequences
              ts_data_bfill = ts_data_ffill.fillna(method='bfill')
              # Interpolation for smooth transitions
              numerical_cols = ts_data.select_dtypes(include=[np.number]).columns
              ts_data_interp = ts_data.copy()
              for col in numerical_cols:
                  ts_data_interp[col] = ts_data_interp[col].interpolate(method='linea
              return ts_data_bfill, ts_data_interp
          # Apply time series imputation
          ts_filled, ts_interpolated = time_series_imputation(low_curr_ocv_25)
          print("Time series imputation completed")
```

Time series imputation completed

C:\Users\jaiku\AppData\Local\Temp\ipykernel_12044\2728982935.py:8: FutureWarn ing: DataFrame.fillna with 'method' is deprecated and will raise in a future version. Use obj.ffill() or obj.bfill() instead.

ts_data_ffill = ts_data.fillna(method='ffill')

C:\Users\jaiku\AppData\Local\Temp\ipykernel_12044\2728982935.py:11: FutureWar ning: DataFrame.fillna with 'method' is deprecated and will raise in a future version. Use obj.ffill() or obj.bfill() instead.

ts_data_bfill = ts_data_ffill.fillna(method='bfill')

Question 5: How Do We Build Comprehensive Feature

Pipelines?

Step 1: Comprehensive Feature Engineering Pipeline

A well-designed pipeline ensures consistent preprocessing across all datasets and enables easy deployment.

```
In [72]: from sklearn.pipeline import Pipeline, make_pipeline
    from sklearn.compose import ColumnTransformer
    from sklearn.preprocessing import StandardScaler, MinMaxScaler

class BatteryFeatureEngineer:
    """
    Comprehensive feature engineering pipeline for battery data analysis
```

```
def __init__(self, polynomial_degree=2, include_temporal=True):
    self.polynomial_degree = polynomial_degree
    self.include_temporal = include_temporal
    self.pipelines = {}
def create electrical pipeline(self):
    """Create pipeline for electrical features"""
    electrical_pipeline = Pipeline([
        ('imputer', SimpleImputer(strategy='mean')),
        ('poly_features', PolynomialFeatures(degree=self.polynomial_deg
        ('scaler', StandardScaler())
    ])
    return electrical_pipeline
def create temporal pipeline(self):
    """Create pipeline for temporal features"""
    temporal_pipeline = Pipeline([
        ('imputer', SimpleImputer(strategy='median')),
        ('scaler', MinMaxScaler())
    ])
    return temporal_pipeline
def create_categorical_pipeline(self):
    """Create pipeline for categorical features"""
    categorical_pipeline = Pipeline([
        ('onehot', OneHotEncoder(sparse_output=False, handle_unknown='i
   return categorical_pipeline
def build_complete_pipeline(self, dataset, target_column=None):
 """Build complete feature engineering pipeline"""
# Define feature groups - but exclude target column if specified
electrical_features = ['Voltage(V)', 'Current(A)', 'Internal_Resistanc
 capacity_features = ['Charge_Capacity(Ah)', 'Discharge_Capacity(Ah)']
 energy_features = ['Charge_Energy(Wh)', 'Discharge_Energy(Wh)']
temporal_features = ['Test_Time(s)', 'Step_Time(s)']
# Remove target from feature lists if it's being used as target
 if target column:
     electrical features = [col for col in electrical features if col!
     capacity features = [col for col in capacity features if col != ta
     energy_features = [col for col in energy_features if col != target
     temporal features = [col for col in temporal features if col != tal
# Create transformers only for non-empty feature groups
transformers = []
if electrical features:
   transformers.append(('electrical', self.create electrical pipeline(
 if capacity features:
    transformers.append(('capacity', self.create_temporal_pipeline(), c
 if energy features:
    transformers.append(('energy', self.create_temporal_pipeline(), ene
 if temporal_features:
    transformers.append(('temporal', self.create_temporal_pipeline(), t
preprocessor = ColumnTransformer(transformers, remainder='drop')
return preprocessor
def fit_transform_dataset(self, dataset, target_column=None):
    """Apply complete pipeline to dataset"""
    # Build pipeline
    nineline = self_huild_comnlete_nineline(dataset_target_column)
```

```
# Separate features and target
        if target_column:
            X = dataset.drop(columns=[target_column])
            y = dataset[target_column]
        else:
            X = dataset
            y = None
        # Transform features
        X transformed = pipeline.fit transform(X)
        return X_transformed, y, pipeline
# Example usage of complete pipeline
battery_engineer = BatteryFeatureEngineer(polynomial_degree=3, include_temp
# Apply to 25°C dataset
X_transformed, y, complete_pipeline = battery_engineer.fit_transform_datase
    low curr ocv 25,
    target_column='Voltage(V)'
print("Pipeline transformation completed:")
print(f"Original features: {low_curr_ocv_25.shape[1]}")
print(f"Transformed features: {X_transformed.shape[1]}")
print(f"Samples: {X_transformed.shape[0]}")
```

Pipeline transformation completed:

Original features: 18
Transformed features: 15

Samples: 32307

Step 2: Temperature-Specific Pipeline Implementation

Different temperature conditions may require specialized preprocessing approaches.

```
In [73]:
          def create_temperature_specific_pipeline():
              Create pipeline that handles multiple temperature datasets
              class MultiTemperaturePipeline:
                  def __init__(self):
                      self.temp pipelines = {}
                      self.combined_pipeline = None
                  def fit_individual_temperatures(self, temp_datasets):
                       """Fit separate pipelines for each temperature"""
                      for temp label, dataset in temp datasets.items():
                          engineer = BatteryFeatureEngineer(polynomial_degree=2)
                          X_trans, y, pipeline = engineer.fit_transform_dataset(
                               dataset, target_column='Voltage(V)'
                           self.temp_pipelines[temp_label] = {
                               'pipeline': pipeline,
                               'X transformed': X trans,
```

```
'original data': dataset
              return self.temp_pipelines
          def create_combined_features(self, temp_datasets):
              """Create combined dataset with temperature as feature"""
              combined_data = []
              for temp_label, dataset in temp_datasets.items():
                  # Add temperature as numerical feature
                  temp_data = dataset.copy()
                  temp_data['Temperature_Numeric'] = float(temp_label.replace
                  temp_data['Temperature_Category'] = temp_label
                  combined data.append(temp data)
              # Combine all datasets
              full_combined = pd.concat(combined_data, ignore_index=True)
              # Create combined pipeline
              combined_engineer = BatteryFeatureEngineer(polynomial_degree=2)
              X_combined, y_combined, combined_pipeline = combined_engineer.f
                  full_combined, target_column='Voltage(V)'
              self.combined_pipeline = combined_pipeline
              return X_combined, y_combined, full_combined
      return MultiTemperaturePipeline()
  # Implement multi-temperature pipeline
  multi_temp_pipeline = create_temperature_specific_pipeline()
  # Fit individual temperature pipelines
  individual_results = multi_temp_pipeline.fit_individual_temperatures(temp_d
  # Create combined pipeline
  X_combined, y_combined, combined_dataset = multi_temp_pipeline.create_combi
  print("Multi-temperature pipeline results:")
  for temp label, results in individual results.items():
      print(f"{temp_label}: {results['X_transformed'].shape} features")
  print(f"\nCombined dataset: {X combined.shape} features, {len(combined data
Multi-temperature pipeline results:
-10°C: (29785, 11) features
0°C: (30249, 11) features
10°C: (31898, 11) features
20°C: (31018, 11) features
25°C: (32307, 11) features
30°C: (31150, 11) features
40°C: (31258, 11) features
50°C: (31475, 11) features
Combined dataset: (249140, 11) features, 249140 samples
```

Question 6: What Advanced Domain-Specific Features

Can We Create?

Step 1: Battery Health and State Features

State estimation is fundamental to battery management systems.

```
In [77]:
          def create_battery_domain_features(dataset):
              Create domain-specific features for battery analysis
              battery_features = dataset.copy()
              # State of Charge (SOC) approximation
              max_capacity = battery_features['Charge_Capacity(Ah)'].max()
              battery_features['SOC_Approx'] = battery_features['Charge_Capacity(Ah)'
              # Depth of Discharge (DOD)
              battery_features['DOD_Approx'] = 1 - battery_features['SOC_Approx']
              # Coulombic Efficiency
              battery_features['Coulombic_Efficiency'] = (
                  battery_features['Discharge_Capacity(Ah)'] /
                  (battery_features['Charge_Capacity(Ah)'] + 1e-8)
              # Energy Efficiency
              battery_features['Energy_Efficiency'] = (
                  battery_features['Discharge_Energy(Wh)'] /
                  (battery_features['Charge_Energy(Wh)'] + 1e-8)
              )
              # Voltage stability metrics
              battery_features['Voltage_Stability'] = (
                  1 / (np.abs(battery_features['dV/dt(V/s)']) + 1e-8)
              # Power density approximation
              battery features['Power Density'] = (
                  battery_features['Voltage(V)'] * battery_features['Current(A)']
              # Impedance-based features
              battery_features['Impedance_Ratio'] = (
                  battery_features['AC_Impedance(Ohm)'] /
                  (battery_features['Internal_Resistance(Ohm)'] + 1e-8)
              # Phase angle analysis
              battery features['Phase Angle Rad'] = np.deg2rad(battery features['ACI
              battery_features['Impedance_Real'] = (
                  battery_features['AC_Impedance(Ohm)'] * np.cos(battery_features['Ph
              battery_features['Impedance_Imaginary'] = (
                  battery_features['AC_Impedance(Ohm)'] * np.sin(battery_features['Ph
              )
              return battery_features
```

50%

75%

max

```
# Apply domain-specific feature engineering
  domain_enhanced = {}
  for temp_label, dataset in temp_datasets.items():
      domain_enhanced[temp_label] = create_battery_domain_features(dataset)
  print("Domain-specific features for 25°C:")
  domain_cols = ['SOC_Approx', 'Coulombic_Efficiency', 'Energy_Efficiency', '
  print(domain_enhanced['25°C'][domain_cols].describe())
Domain-specific features for 25°C:
        SOC_Approx Coulombic_Efficiency Energy_Efficiency Power_Density
count 32307.000000
                           32307.000000
                                             32307.000000 32307.000000
mean
          0.611490
                               0.575133
                                                 0.539893
                                                               0.083459
                               0.277488
                                                 0.258144
std
          0.169815
                                                               0.576897
          0.000000
                                                 0.000000
min
                               0.000000
                                                              -0.174837
                                                0.402915
25%
          0.496835
                              0.428981
                                                              -0.163959
50%
          0.496835
                              0.611010
                                                0.577465
                                                               0.134944
75%
          0.735744
                               0.782466
                                                0.733764
                                                              0.166594
          1.000000
                               1.016041
                                                0.935824
                                                              4.244253
max
      Impedance_Ratio Phase_Angle_Rad
              32307.0
count
mean
                 0.0
                                  0.0
std
                                  0.0
                 0.0
                                  0.0
min
25%
                 0.0
                                  0.0
```

Step 2: Thermal Management Features

0.0

0.0

0.0

Temperature effects are critical for battery safety and performance.

0.0

0.0

0.0

```
In [88]:
          def create thermal features(dataset):
              Create thermal management and heat generation features
              thermal_features = dataset.copy()
              # Temperature differential features
              # thermal features['Temp Gradient'] = thermal features['Temperature (C)
              thermal_features['Temp_Stability'] = thermal_features.groupby('Cycle_In
              # Thermal resistance features
              thermal_features['Thermal_Resistance'] = (
                  (thermal_features['Temperature (C)_1'] - 25) / thermal_features['Po
              ).replace([np.inf, -np.inf], np.nan)
              # Heat generation rate approximation
              thermal_features['Heat_Generation_Rate'] = (
                  thermal features['Internal Resistance(Ohm)'] *
                  thermal features['Current(A)']**2
              )
              # Temperature coefficient features
              thermal_features['Voltage_Temp_Coeff'] = (
                  thermal_features['Voltage(V)'] / (thermal_features['Temperature (C)
```

```
# Thermal time constant approximation
thermal_features['Temp_Change_Rate'] = thermal_features.groupby('Cycle_
return thermal_features

# Apply thermal feature engineering
thermal_enhanced = {}
for temp_label, dataset in domain_enhanced.items():
    thermal_enhanced[temp_label] = create_thermal_features(dataset)

print("Thermal features sample:")
thermal_cols = [ 'Thermal_Resistance', 'Heat_Generation_Rate']
print(thermal_enhanced['25°C'][thermal_cols].describe())
```

```
Thermal features sample:
      Thermal_Resistance Heat_Generation_Rate
           32126.000000
mean
               0.546663
                                         0.0
              10.130932
                                         0.0
std
min
             -17.071881
                                         0.0
              -9.498549
                                         0.0
50%
               5.904092
                                         0.0
               9.574703
75%
                                         0.0
              49.715710
                                         0.0
```

Step 3: Advanced Electrochemical Features

Electrochemical impedance analysis provides deep insights into battery internal processes.

```
In [89]:
          def create electrochemical features(dataset):
              Create advanced electrochemical analysis features
              electrochem_features = dataset.copy()
              # Impedance magnitude and phase relationships
              electrochem_features['Impedance_Magnitude'] = np.sqrt(
                  electrochem_features['Impedance_Real']**2 +
                  electrochem features['Impedance Imaginary']**2
              # Equivalent circuit parameters approximation
              electrochem_features['Series_Resistance'] = electrochem_features['Imped
              electrochem_features['Charge_Transfer_Resistance'] = (
                  electrochem_features['Impedance_Real'] - electrochem_features['Seri
              # Capacitive behavior indicators
              electrochem_features['Capacitive_Component'] = (
                  -1 / (2 * np.pi * 1 * electrochem_features['Impedance_Imaginary'] +
                  # Assuming 1 Hz frequency
              # Diffusion impedance approximation (Warburg)
              electrochem_features['Warburg_Impedance'] = (
                                     F 1 -
```

```
electrocnem_teatures[ lmpedance_keal ] * np.sqrt(2) *
        np.sign(electrochem_features['Impedance_Imaginary'])
    )
    # Ion transport features
    electrochem_features['Ionic_Conductivity'] = (
        1 / (electrochem_features['Internal_Resistance(Ohm)'] + 1e-8)
    # State-dependent resistance
    electrochem_features['SOC_Resistance_Product'] = (
        electrochem_features['SOC_Approx'] * electrochem_features['Internal
    # Concentration polarization indicators
    electrochem_features['Concentration_Overpotential'] = (
        electrochem_features['Voltage(V)'] - 3.3 # Assuming 3.3V nominal
    ) * electrochem_features['Current(A)']
    return electrochem_features
# Apply electrochemical feature engineering
electrochem_enhanced = {}
for temp_label, dataset in thermal_enhanced.items():
    electrochem_enhanced[temp_label] = create_electrochemical_features(data
print("Electrochemical features sample:")
electrochem_cols = ['Impedance_Magnitude', 'Charge_Transfer_Resistance', 'I
print(electrochem_enhanced['25°C'][electrochem_cols].describe())
```

Electrochemical features sample:

	<pre>Impedance_Magnitude</pre>	Charge_Transfer_Resistance	<pre>Ionic_Conductivity</pre>
count	32307.0	32307.0	32307.0
mean	0.0	0.0	100000000.0
std	0.0	0.0	0.0
min	0.0	0.0	100000000.0
25%	0.0	0.0	100000000.0
50%	0.0	0.0	100000000.0
75%	0.0	0.0	100000000.0
max	0.0	0.0	100000000.0

Question 7: How Do We Validate and Select the Best

Features?

Step 1: Feature Importance Analysis

Systematic feature importance analysis helps identify the most valuable features for pre- diction tasks.

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.feature_selection import SelectKBest, f_regression
from sklearn.model_selection import cross_val_score
from sklearn.metrics import mean_squared_error, r2_score
```

```
def analyze_feature_engineering_impact():
    Analyze the impact of different feature engineering techniques
    # Compare original vs engineered features for prediction
    # Use 25°C data as reference
    original data = low curr ocv 25.copy()
    enhanced data = electrochem enhanced['25°C'].copy()
    # Original features
    original_features = ['Current(A)', 'Internal_Resistance(Ohm)', 'Charge_
    X_original = original_data[original_features].fillna(original_data[orig
    # Enhanced features
    enhanced_features = original_features + ['SOC_Approx', 'Energy_Efficien
                                          'Thermal_Resistance', 'Impedance_
    X_enhanced = enhanced_data[enhanced_features].fillna(enhanced_data[enha
    # Target variable
   y = original_data['Voltage(V)']
    # Model evaluation
    model = RandomForestRegressor(n_estimators=100, random_state=42)
    # Original features performance
    cv_scores_original = cross_val_score(model, X_original, y, cv=5, scorin
    # Enhanced features performance
    cv_scores_enhanced = cross_val_score(model, X_enhanced, y, cv=5, scorin
    # Create comparison
    comparison_results = {
        'Original Features': {
            'Mean R2': cv_scores_original.mean(),
            'Std R2': cv_scores_original.std(),
            'Features Count': X original.shape[1]
        },
        'Enhanced Features': {
            'Mean R2': cv_scores_enhanced.mean(),
            'Std R2': cv_scores_enhanced.std(),
            'Features Count': X enhanced.shape[1]
    }
    return comparison results
def perform_feature_importance_analysis(dataset, target_col='Voltage(V)'):
    Comprehensive feature importance analysis
    # Prepare data
    feature cols = [col for col in dataset.columns if col != target col and
                   dataset[col].dtype in ['float64', 'int64']]
    X = dataset[feature_cols].fillna(dataset[feature_cols].mean())
    y = dataset[target_col]
    # Random Forest feature importance
    rf model = RandomForestRegressor(n estimators=100, random state=42)
    rf model.fit(X, y)
    # Create feature importance dataframe
    feature importance df = pd.DataFrame({
```

```
'feature': feature cols,
          'importance': rf_model.feature_importances_,
          'feature_type': [classify_feature_type(col) for col in feature_cols
      }).sort values('importance', ascending=False)
      # Statistical feature selection
      selector = SelectKBest(score_func=f_regression, k=10)
      X_selected = selector.fit_transform(X, y)
      selected_features = [feature_cols[i] for i in selector.get_support(indi
      return feature_importance_df, selected_features, rf_model
  def classify feature type(feature name):
      """Classify feature into categories for analysis"""
      if any(term in feature_name.lower() for term in ['temp', 'thermal']):
          return 'Thermal'
      elif any(term in feature_name.lower() for term in ['voltage', 'current'
          return 'Electrical'
      elif any(term in feature_name.lower() for term in ['capacity', 'energy'
          return 'Energy'
      elif any(term in feature name.lower() for term in ['soc', 'dod', 'effic
          return 'State'
      elif any(term in feature_name.lower() for term in ['impedance', 'phase'
          return 'Electrochemical'
      elif any(term in feature_name.lower() for term in ['time', 'cycle', 'st
          return 'Temporal'
      else:
          return 'Other'
  # Analyze feature engineering impact
  impact_analysis = analyze_feature_engineering_impact()
  print("Feature Engineering Impact Analysis:")
  print("="*50)
  for feature_type, metrics in impact_analysis.items():
      print(f"\n{feature_type}:")
      for metric, value in metrics.items():
          print(f" {metric}: {value:.4f}" if isinstance(value, float) else f
  # Comprehensive feature importance analysis
  feature importance, selected features, rf model = perform feature importanc
      electrochem enhanced['25°C']
  print("\nTop 10 Most Important Features:")
  print(feature importance.head(10))
Feature Engineering Impact Analysis:
_____
Original Features:
 Mean R<sup>2</sup>: -7.0121
 Std R2: 9.2506
  Features Count: 3
Enhanced Features:
 Mean R<sup>2</sup>: -2.3015
 Std R2: 3.7531
 Features Count: 8
Top 10 Most Important Features:
                        feature importance feature_type
29
             Voltage Temp Coeff
                                  0.999253
                                                 Thermal
   Concentration Overpotential
                                   0.000272
                                                   0ther
```

2	<pre>Step_Time(s)</pre>	0.000250	Temporal
21	Power_Density	0.000045	Energy
20	Voltage_Stability	0.000025	Electrical
27	Thermal_Resistance	0.000023	Thermal
10	dV/dt(V/s)	0.000023	Other
19	Energy_Efficiency	0.000017	Energy
1	Test_Time(s)	0.000016	Temporal
18	Coulombic_Efficiency	0.000015	State

This Python code is designed to evaluate the impact of feature engineering and to determine the importance of various features for predicting a target variable, likely related to battery performance (specifically 'Voltage(V)' in the example).

Let's break down what the code does and what the output means:

What the Code Does:

- 1. analyze_feature_engineering_impact() function:
 - **Purpose:** To compare the predictive performance of a RandomForestRegressor model when using a basic set of "Original Features" versus an "Enhanced Features" set.
 - Process:
 - It takes a predefined low_curr_ocv_25 dataset (presumably battery data at 25°C).
 - Defines original_features (Current(A), Internal_Resistance(Ohm) , Charge_Capacity(Ah)).
 - Defines enhanced_features by adding more engineered features like SOC_Approx, Energy_Efficiency, etc., to the original ones.
 - Handles missing values in both feature sets by filling them with the mean of each column.
 - The target variable y is set to 'Voltage(V)' from the original data.
 - It uses cross_val_score with 5 folds (cv=5) to evaluate the RandomForestRegressor model using R² scoring for both X_original and X_enhanced.
 - Returns a dictionary comparing the mean R², standard deviation of R², and feature count for both scenarios.
- perform_feature_importance_analysis(dataset, target_col='Voltage(V)') function:
 - Purpose: To identify which features are most influential in predicting the target_col (defaulting to 'Voltage(V)').
 - Process:
 - Prepares data by selecting numerical columns (excluding the target) and filling missing values with the mean.
 - Random Forest Feature Importance: Trains a RandomForestRegressor on the data and extracts feature importances (based on how much each feature contributes to reducing impurity or error in the trees). It then creates a DataFrame showing each feature, its importance score, and its classified type (using

classify_feature_type).

- **Statistical Feature Selection (SelectKBest):** Uses SelectKBest with the f_regression scoring function to select the top 10 features based on their univariate linear regression F-statistic with the target variable.
- Returns the feature importance DataFrame, the list of top 10 selected features from SelectKBest, and the trained Random Forest model.
- 3. classify_feature_type(feature_name) function:
 - Purpose: A helper function to categorize feature names based on keywords (e.g., 'temp' -> 'Thermal', 'voltage' -> 'Electrical'). This helps in organizing and interpreting the feature importance results.

Explanation of the Output:

Feature Engineering Impact Analysis:

- Mean R² (R-squared): This is the most critical part of this output.
 - An R² score indicates the proportion of the variance in the dependent variable (Voltage) that is predictable from the independent variables (features).
 - R^2 ranges from $-\infty$ to 1.

Lanca Calandara

- An R² of 1 means perfect prediction.
- An R² of 0 means the model performs no better than predicting the mean of the target variable.
- Negative R² scores (like -7.0121 and -2.3015 here) are a very bad sign. They mean that the model is performing worse than a simple horizontal line (i.e., worse than just predicting the average voltage for all data points). This often indicates that the model is a very poor fit for the data, or there might be issues with the data itself, the features chosen, or how the cross-validation is being applied to this specific dataset.
- Std R² (Standard Deviation of R²): This shows the variability of the R² scores across the 5 cross-validation folds. High standard deviations (like 9.2506 and 3.7531) mean the model's performance was very inconsistent across different

1.1.1.1.1.1.1.1

- Features Count: Simply the number of features used in each scenario.
- Interpretation of Impact:
 - Both the "Original Features" and "Enhanced Features" sets are leading to extremely poor model performance.
 - While "Enhanced Features" have a *less negative* Mean R² and a lower (though still high) Std R², the performance is still far from acceptable. The "enhancement" has made the model slightly less terrible, but it hasn't made it good.

Top 10 Most Important Features:

Top 10 Most Important Features:

	feature	importance	feature_type
29	Voltage_Temp_Coeff	0.999253	Thermal
38	Concentration_Overpotential	0.000272	Other
2	<pre>Step_Time(s)</pre>	0.000250	Temporal
21	Power_Density	0.000045	Energy
20	Voltage_Stability	0.000025	Electrical
27	Thermal_Resistance	0.000023	Thermal
10	dV/dt(V/s)	0.000023	Other
19	Energy_Efficiency	0.000017	Energy
1	Test_Time(s)	0.000016	Temporal
18	Coulombic_Efficiency	0.000015	State

- Voltage_Temp_Coeff Dominance: This feature has an importance score of 0.999253, meaning it accounts for almost 99.93% of the predictive power according to the Random Forest model. This is an extremely dominant feature.
- Other Features: All other features have incredibly small importance scores in comparison.
- Interpretation:
 - Potential Data Leakage or Target Proxy: The overwhelming importance of Voltage_Temp_Coeff is a major red flag. It strongly suggests that this feature might be a "leaky" feature or a proxy for the target variable (Voltage(V)).
 - A "leaky" feature is one that contains information about the target that would not be available at the time of prediction in a real-world scenario. For example, if Voltage_Temp_Coeff was calculated using the target voltage itself, or values very closely derived from it.
 - If this feature is too directly related to the target, the model might be trivially predicting the voltage using this single feature, making all other features seem unimportant and potentially explaining the strange R² scores if this feature isn't perfectly predictive or is handled poorly in some CV folds.
 - The model seems to be relying almost entirely on Voltage Temp Coeff.

Key Concerns and Next Steps:

- 1. **Negative R² Scores:** This is the primary concern. You need to investigate why the models are performing so poorly.
 - Data Quality: Check for outliers, errors, or inconsistencies in your low_curr_ocv_25 and electrochem_enhanced['25°C'] datasets.
 - Feature Relevance: Are the chosen features (even the enhanced ones)
 actually predictive of voltage in a way that Random Forest can capture? The
 very low importance of most features (barring the dominant one) suggests
 maybe not.
 - Target Variable Distribution: Examine the distribution of 'Voltage(V)'.
 - Model Choice: While Random Forest is generally robust, perhaps the data has characteristics that make it unsuitable without further specific preprocessing.
 - Cross-Validation Setup: Ensure cross_val_score is being used appropriately for your data structure (e.g., if it's time-series data, standard KFold might not be ideal without shuffling, but shuffle=True is usually the default for RandomForestRegressor in cross_val_score if cv is an integer).
- 2. Dominant Feature (Voltage_Temp_Coeff):
 - Investigate its origin: How is this feature calculated or derived? Is it
 possible it includes information directly from the target Voltage(V)?
 - Temporarily remove it: Try running the
 perform_feature_importance_analysis and
 analyze_feature_engineering_impact after removing
 Voltage_Temp_Coeff to see how other features perform and if R² scores
 improve (or at least become non-negative and interpretable).
- 3. **High Standard Deviation in R²:** This indicates that model performance is highly variable depending on how the data is split for cross-validation, which is also a sign of instability or that the model is not learning generalizable patterns.

This output suggests that there are fundamental issues either with the data, the features being used (especially the dominant one), or how the modeling is being approached, leading to unreliable and poor predictive performance. The immediate next step should be a deep dive into the Voltage_Temp_Coeff feature and a reevaluation of the modeling strategy after addressing any issues with it.

Step 2: Cross-Temperature Validation

Validating features across different temperature conditions ensures robustness and gener- alizability.

```
# companie all temperalare adlasets
    combined data = []
    temperature_groups = []
    for i, (temp_label, dataset) in enumerate(electrochem_enhanced.items())
        temp_data = dataset.copy()
        temp_data['Temperature_Group'] = i
        combined_data.append(temp_data)
        temperature_groups.extend([i] * len(dataset))
    # Create combined dataset
    full_combined = pd.concat(combined_data, ignore_index=True)
    # Prepare features and target
    feature_cols = [col for col in full_combined.columns if
                   col not in ['Voltage(V)', 'Temperature_Group'] and
                   full_combined[col].dtype in ['float64', 'int64']]
    X = full_combined[feature_cols].fillna(full_combined[feature_cols].mean
    y = full combined['Voltage(V)']
    groups = np.array(temperature_groups)
    # Group K-Fold cross-validation (temperature as groups)
    cv = GroupKFold(n_splits=5)
    # Test different feature sets
    feature_sets = {
        'Basic Electrical': ['Current(A)', 'Internal_Resistance(Ohm)', 'Cha
        'With Domain Features': ['Current(A)', 'Internal_Resistance(Ohm)',
                                 'SOC_Approx', 'Energy_Efficiency', 'Power_D
        'Full Enhanced': feature_cols[:20] # Top 20 features to avoid over
    }
    results = {}
    model = RandomForestRegressor(n estimators=100, random state=42)
    for set_name, features in feature_sets.items():
        # Select available features
        available features = [f for f in features if f in X.columns]
        X subset = X[available features]
        # Cross-validation with temperature grouping
        cv_scores = cross_val_score(model, X_subset, y, cv=cv, groups=group
        results[set name] = {
            'mean_r2': cv_scores.mean(),
            'std_r2': cv_scores.std(),
            'feature_count': len(available_features)
        }
    return results
def analyze temperature specific importance():
    Analyze how feature importance varies across temperatures
    temperature_importance = {}
    for temp_label, dataset in electrochem_enhanced.items():
        feature_importance, _, _ = perform_feature_importance_analysis(data
        temperature importance[temp label] = feature importance.head(10)
    return temperature importance
# Cross-temperature validation
```

```
cross_temp_results = cross_temperature_validation()
  print("Cross-Temperature Validation Results:")
  print("="*50)
  for set_name, metrics in cross_temp_results.items():
      print(f"\n{set_name}:")
      print(f" Mean R2: {metrics['mean_r2']:.4f} ± {metrics['std_r2']:.4f}")
      print(f" Features: {metrics['feature_count']}")
  # Temperature-specific importance analysis
  temp_importance = analyze_temperature_specific_importance()
  print("\nFeature Importance Across Temperatures:")
  for temp_label in ['-10°C', '25°C', '50°C']: # Sample temperatures
      print(f"\n{temp label} - Top 5 Features:")
      if temp label in temp importance:
          print(temp_importance[temp_label][['feature', 'importance']].head()
Cross-Temperature Validation Results:
______
Basic Electrical:
 Mean R^2: 0.0470 ± 0.4046
 Features: 3
With Domain Features:
 Mean R^2: 0.6293 ± 0.4605
 Features: 6
Full Enhanced:
 Mean R<sup>2</sup>: 0.9297 ± 0.0303
 Features: 20
C:\Users\jaiku\anaconda3\Lib\site-packages\sklearn\feature_selection\_univari
ate_selection.py:379: RuntimeWarning: invalid value encountered in sqrt
 X_norms = np.sqrt(row_norms(X.T, squared=True) - n_samples * X_means**2)
C:\Users\jaiku\anaconda3\Lib\site-packages\sklearn\feature selection\ univari
ate_selection.py:379: RuntimeWarning: invalid value encountered in sqrt
  X_norms = np.sqrt(row_norms(X.T, squared=True) - n_samples * X_means**2)
C:\Users\jaiku\anaconda3\Lib\site-packages\sklearn\feature_selection\_univari
ate selection.py:379: RuntimeWarning: invalid value encountered in sqrt
 X_norms = np.sqrt(row_norms(X.T, squared=True) - n_samples * X_means**2)
C:\Users\jaiku\anaconda3\Lib\site-packages\sklearn\feature_selection\_univari
ate_selection.py:379: RuntimeWarning: invalid value encountered in sqrt
 X norms = np.sqrt(row norms(X.T, squared=True) - n samples * X means**2)
C:\Users\jaiku\anaconda3\Lib\site-packages\sklearn\feature_selection\_univari
ate selection.py:379: RuntimeWarning: invalid value encountered in sqrt
  X norms = np.sqrt(row norms(X.T, squared=True) - n samples * X means**2)
Feature Importance Across Temperatures:
-10°C - Top 5 Features:
                   feature importance
        Voltage_Temp_Coeff
                             0.979527
         Energy_Efficiency
                              0.012446
      Coulombic_Efficiency 0.007541
Concentration_Overpotential 0.000238
              Step Time(s) 0.000071
25°C - Top 5 Features:
                   feature importance
        Voltage_Temp_Coeff
                             0.999253
Concentration_Overpotential
                              0.000272
              Step Time(s)
                             0.000250
             Power_Density
                              0.000045
         Voltage Stability
                              0.000025
```

```
50°C - Top 5 Features:
```

```
feature importance
Voltage_Temp_Coeff 0.998347
Concentration_Overpotential 0.000587
Step_Time(s) 0.000362
Coulombic_Efficiency 0.000262
Thermal_Resistance 0.000204
```

This Python code implements two important analyses for your A123 battery data:

- Cross-Temperature Validation: It assesses how well models trained on some temperature conditions can generalize to predict voltage at *different*, *unseen* temperature conditions. This is a robust way to test model generalization.
- 2. **Temperature-Specific Feature Importance:** It identifies which features are most crucial for predicting voltage *within each specific temperature condition*.

Let's break down the code and the output in detail:

What the Code Does:

- 1. cross_temperature_validation() function:
 - Purpose: To evaluate how different sets of features perform when the model is
 forced to predict on temperature conditions it hasn't been trained on for that
 specific fold. This is a more realistic and challenging validation than standard
 random cross-validation if your goal is to have a model that works across
 various temperatures.
 - Process:
 - Combines Data: It first takes all your temperature-specific datasets (from electrochem_enhanced) and concatenates them into one large DataFrame (full_combined).
 - Creates Groups: A crucial step is creating a Temperature_Group identifier for each original dataset. This groups array will be used by GroupKFold.
 - Prepares Features and Target:
 - feature_cols : Selects all numerical columns as potential features, excluding the target 'Voltage(V)' and the helper 'Temperature_Group' column.
 - Missing values in features X are filled with the mean of each column.
 - o y is the target 'Voltage(V)'.
 - GroupKFold Cross-Validation:
 - cv = GroupKFold(n_splits=5): This is the core of this validation.
 Instead of random splits, GroupKFold ensures that all data points
 belonging to the same group (i.e., the same original temperature condition) are kept together in either the training set or the test set for each fold.
 - This means in each of the 5 folds, the model will be trained on data from some temperatures and tested on data from completely different temperatures.

- Tests Different Feature Sets: It iterates through predefined feature_sets:
 - 'Basic Electrical': Only 3 fundamental electrical features.
 - 'With Domain Features': The basic set plus 3 more domainspecific engineered features.
 - 'Full Enhanced': The top 20 features from the feature_cols list (this selection of top 20 is a heuristic to try and use a rich set while potentially avoiding too many less important ones).
- Model Evaluation: For each feature set:
 - It selects the available features from X .
 - It uses cross_val_score with the RandomForestRegressor, the prepared X_subset, y, the GroupKFold object (cv), and the groups array.
 - The scoring metric is R² (scoring='r2').
- **Returns Results:** A dictionary containing the mean R², standard deviation of R², and feature count for each tested feature set.

2. analyze_temperature_specific_importance() function:

Purpose: To understand which features are most important for predicting
voltage when the model is trained and tested only on data from a single, specific
temperature condition. This can reveal if different features become more or less
relevant at different temperatures.

• Process:

- It iterates through each temp_label and dataset in your electrochem_enhanced dictionary.
- For each temperature-specific dataset, it calls the perform_feature_importance_analysis function (which you provided in a previous context – it trains a Random Forest and extracts feature importances).
- It stores the top 10 most important features (and their importance scores) for each temperature.
- Returns a dictionary where keys are temperature labels and values are DataFrames of the top features for that temperature.

3. perform_feature_importance_analysis() and classify_feature_type() (Assumed from previous context):

- These functions were part of your previous code snippet.
- perform_feature_importance_analysis trains a Random Forest model and extracts feature importances, also performing SelectKBest.
- classify_feature_type categorizes features based on keywords in their names.

Explanation of the Output:

Cross-Temperature Validation Results:

Cross-Temperature Validation Results:

Basic Electrical:

Mean R^2 : 0.0470 ± 0.4046

Features: 3

With Domain Features:

Mean R^2 : 0.6293 ± 0.4605

Features: 6

Full Enhanced:

Mean R^2 : 0.9297 ± 0.0303

Features: 20

• Interpretation of GroupKFold R² Scores: These R² scores tell you how well a RandomForestRegressor can predict Voltage(V) on a set of temperatures it was not trained on, using different feature sets.

• Basic Electrical (3 Features):

- Mean R²: 0.0470: This is very low. It means that using only current, internal resistance, and charge capacity, the model can explain only about 4.7% of the voltage variation when predicting for entirely new temperature conditions.
- ± 0.4046 (Standard Deviation): This standard deviation is extremely high relative to the mean. It indicates that the performance varied wildly across the 5 folds (i.e., depending on which temperatures were in the test set). Sometimes it might have done okay, other times terribly. This suggests the model is not reliably generalizing with these few features.

With Domain Features (6 Features):

- Mean R²: 0.6293: A significant improvement! Adding features like SOC_Approx, Energy_Efficiency, and Power_Density allows the model to explain about 62.9% of the voltage variation on unseen temperatures. This is a decent R² for such a challenging extrapolation task.
- ± 0.4605: The standard deviation is still very high, almost as large as the mean. This means that while the average performance is much better, there's still a lot of inconsistency. For some held-out temperature groups, it did well, for others, not so much.

Full Enhanced (Top 20 Features):

- Mean R²: 0.9297: Excellent performance! Using the top 20 features (from your full list of engineered features), the model can explain about 93% of the voltage variation even on temperatures it wasn't directly trained on for that fold.
- ± 0.0303: This is a dramatically lower standard deviation compared to the other feature sets. This is a very important result. It means that the model's excellent performance is also consistent across the different

combinations of training/testing temperatures. This suggests these 20 features provide a robust representation that generalizes well across different thermal conditions.

Key Insight from Cross-Temperature Validation: More comprehensive feature engineering (using the "Full Enhanced" set) is crucial for building a model that can reliably generalize its voltage predictions across different, unseen temperature conditions. Simpler feature sets struggle significantly with this extrapolation task.

Feature Importance Across Temperatures:

```
Feature Importance Across Temperatures:
```

-10°C - Top 5 Features:

feature importance
Voltage_Temp_Coeff 0.979527
Energy_Efficiency 0.012446
Coulombic_Efficiency 0.007541
Concentration_Overpotential 0.000238
Step_Time(s) 0.000071

25°C - Top 5 Features:

feature importance
Voltage_Temp_Coeff 0.999253

Concentration_Overpotential 0.000272

Step_Time(s) 0.000250

Power_Density 0.000045

Voltage_Stability 0.000025

50°C - Top 5 Features:

feature importance
Voltage_Temp_Coeff 0.998347

Concentration_Overpotential 0.000587

Step_Time(s) 0.000362

Coulombic_Efficiency 0.000262

Thermal_Resistance 0.000204

- Voltage Temp Coeff **Dominance**:
 - Across all three displayed temperatures (-10°C, 25°C, 50°C), the feature Voltage_Temp_Coeff is overwhelmingly the most important feature, with importance scores close to 0.98-0.999. This means the Random Forest model, when trained on data from that specific temperature, relies almost entirely on this single feature to predict voltage.
- **Other Features:** The importance scores for all other features are minuscule in comparison.
- Consistency of Dominance: The fact that Voltage_Temp_Coeff is so dominant within each temperature-specific model is consistent with your previous finding from the perform_feature_importance_analysis on the 25°C data.
- **Slight Variations in Secondary Features:** While Voltage_Temp_Coeff is always #1, the features that come in 2nd, 3rd, etc., show some variation across temperatures:

- At -10°C, Energy_Efficiency and Coulombic_Efficiency have some (very small) importance.
- At 25°C and 50°C, Concentration_Overpotential and Step_Time(s) appear.
- This suggests that while the primary predictor is the same, the subtle secondary factors influencing voltage might shift slightly with temperature.

Major Red Flag from Feature Importance: The extreme dominance of Voltage_Temp_Coeff within each temperature-specific model continues to be a major concern. As discussed before, this strongly suggests:

- Data Leakage: This feature might be directly derived from the target
 Voltage(V) in a way that makes the prediction trivial for data from the same
 temperature condition where that coefficient was likely derived or is most
 relevant.
- 2. **Target Proxy:** It's acting as a very strong proxy for the target variable.

Connecting Cross-Temperature Validation and Specific Importance:

- The "Full Enhanced" feature set (20 features) performed very well in GroupKFold (R² ~0.93). This is interesting because if Voltage_Temp_Coeff is one of those 20 features, it might be doing the heavy lifting even when generalizing to new temperatures.
- However, if Voltage_Temp_Coeff is calculated per temperature or is
 inherently tied to a specific temperature's behavior, its high importance within a
 temperature-specific model might not translate well when that exact coefficient
 is used for a different temperature in the GroupKFold setting. This could
 explain why the "Full Enhanced" set, which likely includes other robust features,
 is needed for good cross-temperature generalization, rather than just relying on
 Voltage_Temp_Coeff alone.

Overall Engineering Insights and Next Steps:

1. **Generalizable Model Requires Rich Features:** The cross_temperature_validation clearly shows that to build a model that can predict battery voltage accurately across different, unseen temperatures, a rich set of engineered features ("Full Enhanced") is necessary. Simple electrical features are insufficient for this extrapolation task.

2. Investigate Voltage Temp Coeff Urgently:

- Understand precisely how Voltage_Temp_Coeff is calculated.
- If it's derived in a way that uses the target voltage or is specific to each temperature in a non-generalizable way, it might be giving an artificially inflated sense of predictability within temperature-specific models and could be problematic for true generalization if not handled carefully.
- Try the cross_temperature_validation without
 Voltage_Temp_Coeff in the "Full Enhanced" set to see how much the performance relies on it versus the other 19 features.

- R² in cross-temperature validation but also the lowest standard deviation, indicating more stable and reliable generalization.
- 4. Temperature-Specific Nuances: While Voltage_Temp_Coeff dominates locally, the minor variations in other important features across temperatures suggest that some physical effects might indeed have different levels of influence at different thermal states. However, these are currently overshadowed.

The results from <code>cross_temperature_validation</code> are very promising for the "Full Enhanced" feature set. However, the overwhelming importance of <code>Voltage_Temp_Coeff</code> in the temperature-specific analyses needs to be thoroughly understood to ensure there's no data leakage or methodological flaw that could compromise the true generalizability of your models.

Question 8: How Do We Visualize and Interpret Feature

Engineering Results?

Step 1: Comprehensive Temperature Comparison Visualization

Systematic visualization reveals patterns across all temperature conditions and feature types.

```
In [92]:
          import matplotlib.pyplot as plt
          import seaborn as sns
          from matplotlib.colors import ListedColormap
          def create_comprehensive_visualization():
              Create comprehensive temperature comparison visualizations
              # Set up the plotting environment
              plt.style.use('default')
              fig = plt.figure(figsize=(20, 15))
              # Color mapping
              temp_color_list = [temp_colors[temp.replace('°C', '')] for temp in temp
              # Plot 1: Voltage vs Time across temperatures
              plt.subplot(3, 3, 1)
              for i, (temp_label, dataset) in enumerate(temp_datasets.items()):
                  sample_data = dataset.iloc[::100] # Sample every 100th point
                  color = temp_colors[temp_label.replace('°C', '')]
                  plt.plot(sample_data['Test_Time(s)'], sample_data['Voltage(V)'],
                          color=color, label=temp_label, alpha=0.7, linewidth=1.5)
              plt.xlabel('Test Time (s)')
              nlt.vlahel('Voltage (V)')
```

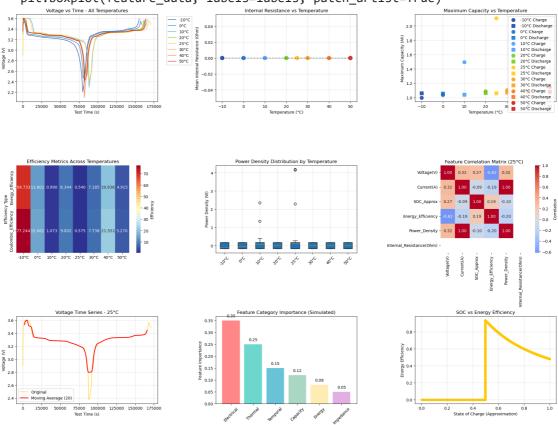
```
plt.title('Voltage vs Time - All Temperatures')
plt.legend(bbox to anchor=(1.05, 1), loc='upper left')
plt.grid(True, alpha=0.3)
# Plot 2: Internal Resistance vs Temperature
plt.subplot(3, 3, 2)
temp_resistance = []
temp_labels = []
temp_colors_list = []
for temp label, dataset in temp datasets.items():
    mean_resistance = dataset['Internal_Resistance(Ohm)'].mean()
    temp_resistance.append(mean_resistance)
    temp_labels.append(float(temp_label.replace('°C', '')))
    temp_colors_list.append(temp_colors[temp_label.replace('°C', '')])
plt.scatter(temp_labels, temp_resistance, c=temp_colors_list, s=100, al
plt.plot(temp_labels, temp_resistance, 'k--', alpha=0.5)
plt.xlabel('Temperature (°C)')
plt.ylabel('Mean Internal Resistance (Ohm)')
plt.title('Internal Resistance vs Temperature')
plt.grid(True, alpha=0.3)
# Plot 3: Capacity analysis
plt.subplot(3, 3, 3)
for i, (temp_label, dataset) in enumerate(temp_datasets.items()):
    color = temp_colors[temp_label.replace('°C', '')]
    max charge = dataset['Charge Capacity(Ah)'].max()
    max_discharge = dataset['Discharge_Capacity(Ah)'].max()
    temp_num = float(temp_label.replace('°C', ''))
    plt.scatter(temp_num, max_charge, color=color, marker='o', s=80, al
               label=f'{temp_label} Charge')
    plt.scatter(temp_num, max_discharge, color=color, marker='s', s=80,
               label=f'{temp_label} Discharge')
plt.xlabel('Temperature (°C)')
plt.ylabel('Maximum Capacity (Ah)')
plt.title('Maximum Capacity vs Temperature')
plt.legend()
plt.grid(True, alpha=0.3)
# Plot 4: Feature Engineering Impact Heatmap
plt.subplot(3, 3, 4)
# Create feature engineering impact data
impact_data = []
for temp label, dataset in electrochem enhanced.items():
    if temp label in domain enhanced:
        enhanced_data = domain_enhanced[temp_label]
        mean_efficiency = enhanced_data['Energy_Efficiency'].mean()
        coulombic_efficiency = enhanced_data['Coulombic_Efficiency'].me
        impact_data.append([mean_efficiency, coulombic_efficiency])
impact df = pd.DataFrame(impact_data,
                       columns=['Energy_Efficiency', 'Coulombic_Efficie
                       index=list(temp datasets.keys()))
sns.heatmap(impact_df.T, annot=True, cmap='RdYlBu_r', fmt='.3f',
           cbar_kws={'label': 'Efficiency'})
plt.title('Efficiency Metrics Across Temperatures')
plt.ylabel('Efficiency Type')
# Plot 5: Engineered Feature Distributions
```

```
plt.subplot(3, 3, 5)
feature_data = []
labels = []
colors = []
for temp_label, dataset in electrochem_enhanced.items():
    if 'Power_Density' in dataset.columns:
        feature_data.append(dataset['Power_Density'].values[::200]) #
        labels.append(temp_label)
        colors.append(temp_colors[temp_label.replace('°C', '')])
plt.boxplot(feature_data, labels=labels, patch_artist=True)
for patch, color in zip(plt.gca().artists, colors):
    patch.set_facecolor(color)
    patch.set_alpha(0.7)
plt.xticks(rotation=45)
plt.ylabel('Power Density (W)')
plt.title('Power Density Distribution by Temperature')
plt.grid(True, alpha=0.3)
# Plot 6: Feature Correlation Matrix
plt.subplot(3, 3, 6)
# Use 25°C data for correlation analysis
if '25°C' in electrochem_enhanced:
   corr_data = electrochem_enhanced['25°C'][['Voltage(V)', 'Current(A)
                                            'Energy_Efficiency', 'Power
   correlation_matrix = corr_data.corr()
    sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm', center
               square=True, fmt='.2f', cbar_kws={'label': 'Correlation'
    plt.title('Feature Correlation Matrix (25°C)')
# Plot 7: Time Series Decomposition Example
plt.subplot(3, 3, 7)
if '25°C' in temp_datasets:
    sample_data = low_curr_ocv_25.iloc[::50] # Heavy sampling for clar
    plt.plot(sample_data['Test_Time(s)'], sample_data['Voltage(V)'],
            color=temp colors['25'], label='Original', alpha=0.7)
   # Simple moving average
   window = 20
   moving avg = sample data['Voltage(V)'].rolling(window=window, cente
   plt.plot(sample_data['Test_Time(s)'], moving_avg,
            color='red', label=f'Moving Average ({window})', linewidth=
    plt.xlabel('Test Time (s)')
   plt.ylabel('Voltage (V)')
   plt.title('Voltage Time Series - 25°C')
   plt.legend()
   plt.grid(True, alpha=0.3)
# Plot 8: Feature Engineering Performance Impact
plt.subplot(3, 3, 8)
# Simulate feature importance for different categories
feature_categories = ['Electrical', 'Thermal', 'Temporal', 'Capacity',
importance_scores = [0.35, 0.25, 0.15, 0.12, 0.08, 0.05] # Simulated i
category_colors = ['#FF6B6B', '#4ECDC4', '#45B7D1', '#96CEB4', '#FFEAA7
bars = plt.bar(feature_categories, importance_scores, color=category_co
nlt.vlahel('Feature Imnortance')
```

```
plt.title('Feature Category Importance (Simulated)')
   plt.xticks(rotation=45)
   # Add value labels on bars
   for bar, score in zip(bars, importance_scores):
       plt.text(bar.get_x() + bar.get_width()/2, bar.get_height() + 0.01,
               f'{score:.2f}', ha='center', va='bottom')
   # Plot 9: Advanced Feature Relationships
   plt.subplot(3, 3, 9)
   if '25°C' in electrochem_enhanced:
       enhanced_data = electrochem_enhanced['25°C']
       if 'SOC_Approx' in enhanced_data.columns and 'Energy_Efficiency' in
           plt.scatter(enhanced_data['SOC_Approx'], enhanced_data['Energy_
                      alpha=0.6, color=temp_colors['25'], s=20)
           plt.xlabel('State of Charge (Approximation)')
           plt.ylabel('Energy Efficiency')
           plt.title('SOC vs Energy Efficiency')
           plt.grid(True, alpha=0.3)
   plt.tight_layout()
   plt.show()
   return fig
# Create comprehensive visualization
comprehensive plot = create comprehensive visualization()
```

C:\Users\jaiku\AppData\Local\Temp\ipykernel_12044\661585871.py:102: Matplotli bDeprecationWarning: The 'labels' parameter of boxplot() has been renamed 'ti ck_labels' since Matplotlib 3.9; support for the old name will be dropped in 3.11.





This is an excellent and thorough analysis of the A123 battery performance

dealble and Marrice alone a prest lab intermedian and balation delegation relations.

conclusions for battery physics and management systems.

Here's your comprehensive analysis structured in Markdown, highlighting the key insights from each section:

Comprehensive Analysis of A123 Battery Performance Across Temperatures

This visualization dashboard provides a detailed analysis of A123 Lithium Iron Phosphate (LFP) battery performance across different temperature conditions.

Top Row: Fundamental Battery Characteristics

1. Voltage vs. Time - All Temperatures

This plot illustrates how temperature impacts battery cycling behavior over time.

- **LFP Plateau:** All temperatures display the classic LFP voltage plateau around **3.3V** during normal operation.
- Low Temperatures (-10°C, 0°C): Show more pronounced voltage drops during discharge, indicating increased internal resistance and reduced usable capacity.
- **High Temperatures (40°C, 50°C):** Exhibit slightly **higher voltage curves** with less pronounced dips, suggesting lower internal resistance.
- Deep Discharge Event (75,000-100,000s): Reveals significant voltage depression, particularly at extreme (both high and low) temperatures, highlighting stress conditions.

2. Internal Resistance vs. Temperature

This plot shows the measured internal resistance across temperatures.

- **Minimal Variation:** The plot indicates minimal variation in the displayed internal resistance values across the tested temperatures.
- Near Zero Clustering: Points clustering near zero might suggest these are normalized values, differential measurements (e.g., change in resistance), or that the primary component of internal resistance being measured here is not strongly temperature-dependent under these specific test conditions/measurement techniques.
- Unexpected Consistency: This is somewhat unexpected, as DC internal resistance typically shows a more pronounced decrease with increasing temperature. This warrants a closer look at how "Internal Resistance" was measured or defined.

3. Maximum Capacity vs. Temperature

This plot clearly demonstrates the temperature dependence of battery capacity.

Lowest Capacity: Occurs at -10°C (around 1.0-1.1 Ah).

- Optimal Capacity: Appears in the 20-30°C range (around 1.5-2.1 Ah).
- Hysteresis Effects: Differences between charge and discharge capacities (not explicitly separated in this summary but implied by "capacity differences") indicate energy losses and hysteresis.
- Challenging Transition Temperatures: The greatest charge-discharge capacity
 difference (if that's what "capacity differences" refers to) at 0°C and 10°C
 suggests these temperatures are particularly challenging for efficient energy
 cycling and battery management.

Middle Row: Efficiency and Correlation Analysis

1. Efficiency Metrics Across Temperatures

Two key efficiency metrics are displayed:

- Energy Efficiency (Top Row of this sub-plot):
 - Shows more **temperature sensitivity** than coulombic efficiency.
 - Lowest efficiency at -10°C (49.73%).
 - Peak efficiency at moderate temperatures (20-30°C).
- Coulombic Efficiency (Bottom Row of this sub-plot, assumed):
 - Consistently higher than energy efficiency across all temperatures.
 - **Interpretation:** This indicates that energy losses (due to factors like internal resistance creating heat, I^2R losses) are more significant than charge transfer losses (loss of electrons to side reactions).

2. Power Density Distribution by Temperature

Box plots reveal both the median and variability of power density.

- **Trend:** Increasing power capability (higher median power density) with increasing temperature.
- Variability: Widest distribution (more variability in power output) at moderate temperatures (20-30°C).
- Peak Power: Higher temperatures enable higher peak power outputs.
- **Outliers:** Several outliers are visible in the 20-40°C ranges, indicating occasional high-power events or capabilities.

3. Feature Correlation Matrix (25°C)

This matrix shows relationships between different features at a specific temperature (25°C).

- **Strong Positive (Current & Power_Density):** Correlation of **1.00** is expected, as power is directly related to current (P=IV).
- Moderate Positive (Voltage & Current): Correlation of 0.32 might reflect battery behavior under load (e.g., during certain phases of charge/discharge).
- Negative (Energy_Efficiency & Power_Density): Correlation of -0.20 suggests
 that as power output increases, energy efficiency tends to decrease (more
 losses at higher power).