```
Last login: Fri Feb  3 14:42:27 on ttys000
(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE
/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE: /Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE: is a directory
(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run.sh
python: can't open file '/Users/rishabhgoel/process_data.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/data_split.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/run_train.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/run_predict
```

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python: can't open file '/Users/rishabhgoel/data_split.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/run_train.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/run_predict.py': [Errno 2] No such file or directory
python: can't open file '/Users/rishabhgoel/data_split.py': [Errno 2] No such file or directory
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/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
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Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run_train.py", line 12, in <module>
    from torchdiffeq import odeint_adjoint as odeint
ModuleNotFoundError: No module named 'torchdiffeq'
Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run_predict.py", line 8, in <module>
    import utils
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ModuleNotFoundError: No module named 'torchdiffeq'
^C
(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % pip3 install torchdiffeq
Collecting torchdiffeq
  Downloading torchdiffeq-0.2.3-py3-none-any.whl (31 kB)
Requirement already satisfied: scipy>=1.4.0 in ./opt/anaconda3/lib/python3.9/site-packages (from torchdiffeq) (1.7.3)
Requirement already satisfied: torch>=1.3.0 in ./opt/anaconda3/lib/python3.9/site-packages (from torchdiffeq) (1.11.0)
Requirement already satisfied: numpy<1.23.0,>=1.16.5 in ./opt/anaconda3/lib/python3.9/site-packages (from scipy>=1.4.0->torchdiffeq) (1.21.5)
Requirement already satisfied: typing-extensions in ./opt/anaconda3/lib/python3.9/site-packages (from torch>=1.3.0->torchdiffeq) (4.3.0)
Installing collected packages: torchdiffeq
Successfully installed torchdiffeq-0.2.3
(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run.sh
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/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run_train.py
Desktop/SupplementaryCode/5fold_models/Neural-ODE/run_train.py --fold 1 --model 1 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:25<00:00,  7.82it/s]
tensor([ 0.2262,  5.2315,  8.9786,  9.3791, 13.0919, 13.3213, 13.5220, 17.2931,
        17.4656], grad_fn=<IndexBackward0>)
tensor([ 5.8156,  0.8816, 16.1310,  0.8871, 19.8420,  3.7824,  0.8870, 20.1590,
         5.8156])

        Epoch 0001 | Training loss 26.023924 | Training R2 -0.761777 | Validation loss 27.330227 | Validation R2 -1.235341
        Best loss 27.330227 | Best epoch 0001

100%|########################################| 672/672 [01:26<00:00,  7.79it/s]
tensor([4.6908, 9.7601, 9.8749, 9.9733], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0002 | Training loss 26.732929 | Training R2 -0.859082 | Validation loss 28.909950 | Validation R2 -1.501221
        Best loss 27.330227 | Best epoch 0001

100%|########################################| 672/672 [01:25<00:00,  7.87it/s]
tensor([ 6.3561, 10.0968, 10.1091, 10.1211], grad_fn=<IndexBackward0>)
tensor([ 2.0678, 51.9320, 15.5760,  5.7433])

        Epoch 0003 | Training loss 25.917587 | Training R2 -0.747408 | Validation loss 27.648657 | Validation R2 -1.287733
        Best loss 27.330227 | Best epoch 0001

100%|########################################| 672/672 [01:25<00:00,  7.85it/s]
tensor([ 7.4450, 10.5858, 10.4464, 10.3043], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 24.462358 | Training R2 -0.556689 | Validation loss 25.198891 | Validation R2 -0.900291
        Best loss 25.198891 | Best epoch 0004

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([13.0975, 17.3474, 16.9537, 16.0470, 20.1991, 19.5002, 17.5652, 21.7773,
        20.6738, 18.5450, 22.9046, 21.6380, 19.2138, 23.4309, 22.0190],
       grad_fn=<IndexBackward0>)
tensor([21.5630, 60.7860, 21.2220,  3.9105, 61.5820, 21.8290,  4.0223, 60.9380,
        21.6020,  3.9807, 62.4120, 22.1240,  4.0767, 60.9140, 21.5630])

        Epoch 0005 | Training loss 21.083540 | Training R2 -0.156358 | Validation loss 24.022093 | Validation R2 -0.726947
        Best loss 24.022093 | Best epoch 0005

100%|########################################| 672/672 [01:26<00:00,  7.77it/s]
tensor([13.8988, 19.9455, 19.2749], grad_fn=<IndexBackward0>)
tensor([ 4.7871, 64.8820, 17.1420])

        Epoch 0006 | Training loss 19.201651 | Training R2 0.040859 | Validation loss 18.415304 | Validation R2 -0.014881
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:26<00:00,  7.77it/s]
tensor([3.8838, 9.2432, 7.8896], grad_fn=<IndexBackward0>)
tensor([2.0948, 9.5297, 2.0948])

        Epoch 0007 | Training loss 20.586771 | Training R2 -0.102508 | Validation loss 24.883312 | Validation R2 -0.852993
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:26<00:00,  7.78it/s]
tensor([14.1825, 24.6263, 22.8973, 21.0740], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0008 | Training loss 19.861233 | Training R2 -0.026166 | Validation loss 24.477762 | Validation R2 -0.793085
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([ 7.3886, 15.2852, 15.0051, 14.7217, 13.5519, 12.6374, 11.4696,  9.7745,
        16.5592, 14.6723, 12.6844], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0009 | Training loss 19.403126 | Training R2 0.020626 | Validation loss 24.256100 | Validation R2 -0.760757
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:26<00:00,  7.74it/s]
tensor([10.1602, 17.5999, 15.7106, 13.1961, 11.3136, 15.0193, 13.6939],
       grad_fn=<IndexBackward0>)
tensor([ 4.1268, 46.3510, 12.0230,  2.1373,  0.5852,  9.7876,  4.1268])

        Epoch 0010 | Training loss 19.802797 | Training R2 -0.020137 | Validation loss 26.308607 | Validation R2 -1.071348
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([17.6132, 29.6599, 27.6050, 23.1010, 31.0644, 29.0582, 25.1882, 31.9336,
        29.8757, 26.0180, 32.3808, 29.9345, 26.2629], grad_fn=<IndexBackward0>)
tensor([16.3580, 60.8840, 20.3170,  2.9673, 63.1460, 21.1430,  3.0879, 62.4800,
        20.9280,  3.0565, 61.7290, 17.8350,  3.0201])

        Epoch 0011 | Training loss 18.058519 | Training R2 0.151661 | Validation loss 20.707491 | Validation R2 -0.283253
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:26<00:00,  7.74it/s]
tensor([15.4383, 24.8883, 22.1746], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0012 | Training loss 17.740986 | Training R2 0.181232 | Validation loss 19.841864 | Validation R2 -0.178209
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:27<00:00,  7.71it/s]
tensor([ 6.3241, 12.5770,  7.8696, 12.4096,  8.1072, 14.2149,  7.8223, 11.2600,
         7.1939, 10.3775,  6.3101,  9.3190,  5.2168, 10.8383,  8.0949,  3.9391,
         9.5080,  6.7120,  2.4917,  5.1752,  0.8842,  6.3916,  3.4883, -0.8772,
         4.6115,  1.6545, -2.7877,  2.6872, -0.3233, -4.8436,  0.6210, -2.4424,
        -7.9419, -1.5844, -4.7004, -9.3802], grad_fn=<IndexBackward0>)
tensor([ 4.3672, 20.9330,  4.1252, 22.0940,  4.3540, 59.3090,  4.3683, 22.1610,
         4.3672, 22.1610,  4.3672, 22.1610,  4.3672, 73.7310, 22.1640,  4.3678,
        73.7110, 22.1610,  4.3672, 22.1610,  4.3672, 73.7440, 22.1650,  4.3681,
        73.7110, 22.1610,  4.3672, 73.7100, 22.1610,  4.3672, 73.7100, 22.1610,
         4.3672, 73.7100, 22.1610,  4.3672])

        Epoch 0013 | Training loss 17.646467 | Training R2 0.189933 | Validation loss 19.356730 | Validation R2 -0.121299
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([ 1.6994, 17.4405, 13.2031, 11.1923, 10.2834, 20.9034, 18.8324, 16.0101,
        15.2836, 23.9429, 21.1242, 19.7191, 17.9639, 25.3872, 23.1988, 20.2987],
       grad_fn=<IndexBackward0>)
tensor([ 0.7684, 22.7900,  2.1049,  0.8118,  0.5042, 22.8300,  5.4673,  0.8133,
         0.5051, 28.9870,  4.3086,  1.6618,  0.5051, 21.5700,  5.1656,  0.7684])

        Epoch 0014 | Training loss 17.502306 | Training R2 0.203115 | Validation loss 19.610004 | Validation R2 -0.150834
```

```
        Best loss 18.415304 | Best epoch 0006

100%|#########################################| 672/672 [01:27<00:00,  7.68it/s]
tensor([11.4615, 22.3707, 18.7303, 12.3394, 19.1679, 15.6442,  9.1946],
       grad_fn=<IndexBackward0>)
tensor([ 5.5479, 51.8750, 15.8080,  2.3393, 50.7150, 15.6200,  2.3116])

        Epoch 0015 | Training loss 18.001534 | Training R2 0.157006 | Validation loss 23.457544 | Validation R2 -0.646730
        Best loss 18.415304 | Best epoch 0006

100%|#########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([26.0862, 36.4665, 34.4420, 31.6990], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0016 | Training loss 17.815872 | Training R2 0.174305 | Validation loss 16.533590 | Validation R2 0.181928
        Best loss 16.533590 | Best epoch 0016

100%|#########################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([20.8729, 27.1115, 26.6857, 26.2577, 25.8270, 24.5116, 29.1832, 27.9320,
        26.6842, 31.0547, 29.7846, 28.5277, 31.9418, 30.2244, 33.5438, 31.7833,
        35.0980, 33.2931, 36.6418, 34.7919, 38.0724, 36.1795, 39.4280, 37.4934,
        40.6823, 38.7079, 41.8330, 39.8208, 42.9237, 40.8747],
       grad_fn=<IndexBackward0>)
tensor([38.1730, 32.4920, 24.8420, 20.1090, 16.9610, 11.5390, 42.3870, 24.3350,
        16.9860, 47.3100, 27.9650, 19.6630, 34.2530, 20.9790, 35.0450, 21.5240,
        35.5990, 21.8790, 36.1540, 22.2220, 36.2560, 22.3030, 36.3190, 22.3450,
        36.2250, 22.2940, 36.0400, 22.1840, 35.9840, 22.1450])

        Epoch 0017 | Training loss 16.692785 | Training R2 0.275125 | Validation loss 17.948978 | Validation R2 0.035867
        Best loss 16.533590 | Best epoch 0016

100%|#########################################| 672/672 [01:40<00:00,  6.72it/s]
tensor([11.4724, 18.0804, 17.5307, 16.9688, 16.3923, 14.5437, 18.8537, 17.8257,
        16.2227, 20.4424, 17.4939, 21.3679, 18.5040, 22.2148, 19.3835, 23.0034,
        20.1774, 23.7119, 20.8788, 24.3830, 21.5363, 25.0216, 22.1581],
       grad_fn=<IndexBackward0>)
tensor([21.3340, 19.2610, 14.4950, 11.2260,  8.9585,  5.3881, 18.6970, 12.5000,
         8.2546, 26.5910, 10.1260, 28.1980, 11.3250, 29.3320, 12.1280, 30.0900,
        12.6640, 30.4370, 12.9750, 30.7340, 13.1890, 30.9350, 13.3310])

        Epoch 0018 | Training loss 16.666876 | Training R2 0.277374 | Validation loss 15.139571 | Validation R2 0.314063
        Best loss 15.139571 | Best epoch 0018

100%|#########################################| 672/672 [01:50<00:00,  6.06it/s]
tensor([ 9.6680, 15.9835,  6.9571, 18.1178, 13.7828], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0019 | Training loss 14.477341 | Training R2 0.454766 | Validation loss 13.607776 | Validation R2 0.445844
        Best loss 13.607776 | Best epoch 0019

100%|#########################################| 672/672 [02:05<00:00,  5.35it/s]
tensor([ 9.4686, 38.3644, 12.2687, 11.5118,  9.2951], grad_fn=<IndexBackward0>)
tensor([ 2.7853, 66.9550,  2.7495,  2.3342,  2.7853])

        Epoch 0020 | Training loss 14.510922 | Training R2 0.452234 | Validation loss 16.810085 | Validation R2 0.154337
        Best loss 13.607776 | Best epoch 0019

100%|#########################################| 672/672 [02:28<00:00,  4.53it/s]
tensor([ 8.5368, 33.8088, 18.8426,  7.7205, 27.9494, 14.5820,  7.0804, 27.8945,
        15.7736,  7.0733, 27.7991, 14.5482,  7.1518, 27.5038, 15.6676,  7.2093,
        27.8395, 15.8780,  7.2429, 27.8744, 15.9120,  7.2845, 27.1735, 14.3810,
         7.5503,  7.2736, 27.7247, 15.8215,  7.3511, 27.2426,  7.5329, 27.9717,
        16.0528,  7.4791], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900, 51.6110, 17.8000,  2.9402,
        52.2210, 18.0080,  2.9745, 52.2510, 18.0190,  2.9764, 50.5100, 15.1680,
         3.3052,  2.8777, 51.7310, 17.8380,  2.9464, 50.4840,  2.8761, 51.7290,
        17.8370,  2.9463])

        Epoch 0021 | Training loss 11.205886 | Training R2 0.673339 | Validation loss 10.361195 | Validation R2 0.678725
        Best loss 10.361195 | Best epoch 0021

100%|#########################################| 672/672 [02:39<00:00,  4.21it/s]
tensor([ 7.2399, 32.7656, 15.4638,  8.0082,  6.0111,  5.5762, 17.2878,  7.8308,
         5.4720, 15.2764,  7.6041,  5.4436,  5.2924], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0022 | Training loss 9.869438 | Training R2 0.746610 | Validation loss 9.603258 | Validation R2 0.724009
        Best loss 9.603258 | Best epoch 0022

100%|#########################################| 672/672 [02:35<00:00,  4.32it/s]
tensor([15.8579, 50.2009, 26.6418, 14.6086, 46.3771, 24.7828, 14.7037, 46.6151,
        14.9483, 46.6064, 25.1501, 15.1815, 46.7140, 25.3345, 15.4388, 46.7163,
        25.5262, 15.7424, 47.2646, 25.5042, 15.9307, 47.3325, 25.6759, 16.1516,
        25.6520, 16.3157, 47.7276, 26.3268, 16.6276, 48.0307, 26.6325],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0023 | Training loss 8.880115 | Training R2 0.794864 | Validation loss 7.997626 | Validation R2 0.808583
        Best loss 7.997626 | Best epoch 0023

100%|#########################################| 672/672 [02:31<00:00,  4.43it/s]
tensor([17.2749, 69.2989, 34.9108, 18.0806, 29.8557, 17.5402, 65.0494, 31.9385,
        17.1078], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317])

        Epoch 0024 | Training loss 7.985860 | Training R2 0.834099 | Validation loss 8.102264 | Validation R2 0.803542
        Best loss 7.997626 | Best epoch 0023

100%|#########################################| 672/672 [02:34<00:00,  4.35it/s]
tensor([11.3186, 17.6525,  7.2354,  5.7471, 42.5767, 15.1930,  9.6660,  6.2997,
         5.1429, 14.7872,  5.7812,  4.6024], grad_fn=<IndexBackward0>)
tensor([17.2550, 16.6050,  5.5696,  2.1836, 53.8670, 17.2450, 10.7980,  5.7840,
         2.2677, 17.4680,  5.8590,  2.2971])

        Epoch 0025 | Training loss 8.279782 | Training R2 0.821662 | Validation loss 9.688253 | Validation R2 0.719102
        Best loss 7.997626 | Best epoch 0023

100%|#########################################| 672/672 [02:43<00:00,  4.12it/s]
tensor([15.5552, 21.2986,  8.9259, 19.4323,  8.8088, 49.8646, 19.4493,  8.6966,
        19.4075,  8.7305, 50.9847, 17.1765,  8.5072, 19.3949,  8.6471, 19.4621,
         8.3514, 19.4284,  8.7043,  7.9715, 19.3271,  7.7307, 19.0096,  7.5651,
        31.6473, 13.4038,  7.8101, 21.1455], grad_fn=<IndexBackward0>)
tensor([23.5920, 20.2570,  2.7573, 21.0380,  2.8637, 70.1770, 21.0260,  2.8620,
        21.0260,  2.8620, 70.1760, 18.0350,  2.8620, 21.0280,  2.8623, 21.0310,
         2.8627, 21.0320,  4.5357,  2.8628, 21.0320,  2.8627, 20.7940,  2.8304,
        37.6000, 12.7810,  2.7564, 23.5920])

        Epoch 0026 | Training loss 6.741351 | Training R2 0.881778 | Validation loss 6.505997 | Validation R2 0.873327
        Best loss 6.505997 | Best epoch 0026

100%|#########################################| 672/672 [02:52<00:00,  3.89it/s]
tensor([ 6.7332, 80.9639, 29.2949, 11.5219,  8.3984, 20.1279,  7.6323, 57.2668,
        22.6112,  8.8510,  6.5061, 63.7430,  5.7285], grad_fn=<IndexBackward0>)
tensor([ 6.1430, 77.5480, 24.0970,  7.7805,  2.9525, 17.9790,  3.0428, 55.8410,
        21.1480,  6.8284,  3.0454, 63.6220,  2.9330])

        Epoch 0027 | Training loss 7.444011 | Training R2 0.855848 | Validation loss 8.489068 | Validation R2 0.784336
        Best loss 6.505997 | Best epoch 0026

100%|#########################################| 672/672 [02:53<00:00,  3.86it/s]
tensor([ 7.7094, 43.7068, 36.5667, 25.8860, 12.6556,  7.2692,  4.5190,  3.7489,
        36.6624, 10.6850,  4.4337,  3.8561, 36.7842, 10.8842,  4.6113,  3.9674],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385])

        Epoch 0028 | Training loss 6.370688 | Training R2 0.894421 | Validation loss 5.628891 | Validation R2 0.905179
        Best loss 5.628891 | Best epoch 0028

100%|#########################################| 672/672 [03:08<00:00,  3.56it/s]
tensor([ 3.2122, 45.6662, 11.4265,  2.6867], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0029 | Training loss 6.405765 | Training R2 0.893255 | Validation loss 6.673342 | Validation R2 0.866726
        Best loss 5.628891 | Best epoch 0028

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(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run.sh
Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/process_data.py", line 7, in <module>
    data_complete = pd.read_csv("/Users/rishabhgoel/Desktop/SupplementaryCode/ExampleData/sim_data.csv", na_values='.')
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/util/_decorators.py", line 311, in wrapper
    return func(*args, **kwargs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/io/parsers/readers.py", line 678, in read_csv
    return _read(filepath_or_buffer, kwds)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/io/parsers/readers.py", line 575, in _read
    parser = TextFileReader(filepath_or_buffer, **kwds)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/io/parsers/readers.py", line 932, in __init__
    self._engine = self._make_engine(f, self.engine)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/io/parsers/readers.py", line 1216, in _make_engine
    self.handles = get_handle(  # type: ignore[call-overload]
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/pandas/io/common.py", line 786, in get_handle
    handle = open(
FileNotFoundError: [Errno 2] No such file or directory: '/Users/rishabhgoel/Desktop/SupplementaryCode/ExampleData/sim_data.csv'
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
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  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
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  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 1 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|#########################################| 672/672 [01:27<00:00,  7.71it/s]
tensor([ 0.2262,  5.2315,  8.9786,  9.3791, 13.0919, 13.3213, 13.5220, 17.2931,
        17.4656], grad_fn=<IndexBackward0>)
tensor([ 5.8156,  0.8816, 16.1310,  0.8871, 19.8420,  3.7824,  0.8870, 20.1590,
         5.8156])

        Epoch 0001 | Training loss 26.023924 | Training R2 -0.761777 | Validation loss 27.330227 | Validation R2 -1.235341
        Best loss 27.330227 | Best epoch 0001

  5%|##1                                      | 35/672 [00:03<00:52, 12.09it/s]  5%|##1                                      | 35/672 [00:03<01:04,  9.84it/s]
Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py", line 94, in <module>
    loss.backward()
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/_tensor.py", line 363, in backward
    torch.autograd.backward(self, gradient, retain_graph, create_graph, inputs=inputs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/autograd/__init__.py", line 173, in backward
    Variable._execution_engine.run_backward(  # Calls into the C++ engine to run the backward pass
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/autograd/function.py", line 253, in apply
    return user_fn(self, *args)
```

```
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/adjoint.py", line 126, in backward
    aug_state = odeint(
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/odeint.py", line 77, in odeint
    solution = solver.integrate(t)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/solvers.py", line 28, in integrate
    self._before_integrate(t)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/rk_common.py", line 161, in _before_integrate
    f0 = self.func(t[0], self.y0)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/nn/modules/module.py", line 1110, in _call_impl
    return forward_call(*input, **kwargs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/misc.py", line 189, in forward
    return self.base_func(t, y)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/nn/modules/module.py", line 1110, in _call_impl
    return forward_call(*input, **kwargs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/misc.py", line 159, in forward
    return self.mul * self.base_func(-t, y)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/nn/modules/module.py", line 1110, in _call_impl
    return forward_call(*input, **kwargs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/misc.py", line 138, in forward
    f = self.base_func(t, _flat_to_shape(y, (), self.shapes))
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/adjoint.py", line 95, in augmented_dynamics
    vjp_t, vjp_y, *vjp_params = torch.autograd.grad(
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/autograd/__init__.py", line 275, in grad
    return Variable._execution_engine.run_backward(  # Calls into the C++ engine to run the backward pass
KeyboardInterrupt

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  df["PTNM"] = df["PTNM"] + 0.2
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Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 1 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
  0%|1                                      | 3/672 [00:00<01:12,  9.18it/s]  0%|1                                          | 3/672 [00:00<01:26,  7.70it/s]
Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py", line 94, in <module>
    loss.backward()
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python: can't open file '/Users/rishabhgoel/Desktop/SupplementaryCode/5fold_models/Neural-ODE/run_predict.py': [Errno 2] No such file or directory
(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run.sh
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 1 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([ 0.2262,  5.2315,  8.9786,  9.3791, 13.0919, 13.3213, 13.5220, 17.2931,
        17.4656], grad_fn=<IndexBackward0>)
tensor([ 5.8156,  0.8816, 16.1310,  0.8871, 19.8420,  3.7824,  0.8870, 20.1590,
         5.8156])

        Epoch 0001 | Training loss 26.023924 | Training R2 -0.761777 | Validation loss 27.330227 | Validation R2 -1.235341
        Best loss 27.330227 | Best epoch 0001
```

```
100%|########################################| 672/672 [01:25<00:00,  7.82it/s]
tensor([4.6908, 9.7601, 9.8749, 9.9733], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0002 | Training loss 26.732929 | Training R2 -0.859082 | Validation loss 28.909950 | Validation R2 -1.501221
        Best loss 27.330227 | Best epoch 0001

100%|########################################| 672/672 [01:26<00:00,  7.77it/s]
tensor([ 6.3561, 10.0968, 10.1091, 10.1211], grad_fn=<IndexBackward0>)
tensor([ 2.0678, 51.9320, 15.5760,  5.7433])

        Epoch 0003 | Training loss 25.917587 | Training R2 -0.747408 | Validation loss 27.648657 | Validation R2 -1.287733
        Best loss 27.330227 | Best epoch 0001

100%|########################################| 672/672 [01:26<00:00,  7.81it/s]
tensor([ 7.4450, 10.5858, 10.4464, 10.3043], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 24.462358 | Training R2 -0.556689 | Validation loss 25.198891 | Validation R2 -0.900291
        Best loss 25.198891 | Best epoch 0004

100%|########################################| 672/672 [01:26<00:00,  7.76it/s]
tensor([13.0975, 17.3474, 16.9537, 16.0470, 20.1991, 19.5002, 17.5652, 21.7773,
        20.6738, 18.5450, 22.9046, 21.6380, 19.2138, 23.4309, 22.0190],
       grad_fn=<IndexBackward0>)
tensor([21.5630, 60.7860, 21.2220,  3.9105, 61.5820, 21.8290,  4.0223, 60.9380,
        21.6020,  3.9807, 62.4120, 22.1240,  4.0767, 60.9140, 21.5630])

        Epoch 0005 | Training loss 21.083540 | Training R2 -0.156358 | Validation loss 24.022093 | Validation R2 -0.726947
        Best loss 24.022093 | Best epoch 0005

100%|########################################| 672/672 [01:26<00:00,  7.73it/s]
tensor([13.8988, 19.9455, 19.2749], grad_fn=<IndexBackward0>)
tensor([ 4.7871, 64.0820, 17.1420])

        Epoch 0006 | Training loss 19.201651 | Training R2 0.040859 | Validation loss 18.415304 | Validation R2 -0.014881
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([3.8838, 9.2432, 7.8896], grad_fn=<IndexBackward0>)
tensor([2.0948, 9.5297, 2.0948])

        Epoch 0007 | Training loss 20.586771 | Training R2 -0.102508 | Validation loss 24.883312 | Validation R2 -0.852993
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:27<00:00,  7.71it/s]
tensor([14.1825, 24.6263, 22.8973, 21.0740], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0008 | Training loss 19.861233 | Training R2 -0.026166 | Validation loss 24.477762 | Validation R2 -0.793085
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:26<00:00,  7.72it/s]
tensor([ 7.3886, 15.2852, 15.0051, 14.7217, 13.5519, 12.6374, 11.4696,  9.7745,
        16.5592, 14.6723, 12.6844], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0009 | Training loss 19.403126 | Training R2 0.020626 | Validation loss 24.256100 | Validation R2 -0.760757
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([10.1602, 17.5999, 15.7106, 13.1961, 11.3136, 15.0193, 13.6939],
       grad_fn=<IndexBackward0>)
tensor([ 4.1268, 46.3510, 12.0230,  2.1373,  0.5852,  9.7876,  4.1268])

        Epoch 0010 | Training loss 19.802797 | Training R2 -0.020137 | Validation loss 26.308607 | Validation R2 -1.071348
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([17.6132, 29.6599, 27.6050, 23.1010, 31.0644, 29.0582, 25.1882, 31.9336,
        29.8757, 26.0180, 32.3808, 29.9345, 26.2629], grad_fn=<IndexBackward0>)
tensor([16.3580, 60.8860, 20.3170,  2.9673, 63.1460, 21.1430,  3.0879, 62.4800,
        20.9280,  3.0565, 61.7290, 17.8350,  3.0201])

        Epoch 0011 | Training loss 18.058519 | Training R2 0.151661 | Validation loss 20.707491 | Validation R2 -0.283253
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([15.4383, 24.8883, 22.1746], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0012 | Training loss 17.740986 | Training R2 0.181232 | Validation loss 19.841864 | Validation R2 -0.178209
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 6.3241, 12.5770,  7.8696, 12.4096,  8.1072, 14.2149,  7.8223, 11.2600,
         7.1939, 10.3775,  6.3101,  9.3190,  5.2168, 10.8383,  8.0949,  3.9391,
         9.5080,  6.7120,  2.4917,  5.1752,  0.8842,  6.3916,  3.4883, -0.8772,
         4.6115,  1.6545, -2.7877,  2.6872, -0.3233, -4.8436,  0.6210, -2.4424,
        -7.0419, -1.5844, -4.7004, -9.3802], grad_fn=<IndexBackward0>)
tensor([ 4.3672, 20.9330,  4.1252, 22.0940,  4.3540, 59.3090,  4.3683, 22.1610,
         4.3672, 22.1610,  4.3672, 22.1610,  4.3672, 73.7310, 22.1640,  4.3678,
        73.7110, 22.1610,  4.3672, 22.1610,  4.3672, 73.7440, 22.1650,  4.3681,
        73.7110, 22.1610,  4.3672, 73.7100, 22.1610,  4.3672, 73.7100, 22.1610,
         4.3672, 73.7100, 22.1610,  4.3672])

        Epoch 0013 | Training loss 17.646467 | Training R2 0.189933 | Validation loss 19.356730 | Validation R2 -0.121299
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 1.6994, 17.4405, 13.2031, 11.1923, 10.2834, 20.9034, 18.8324, 16.0101,
        15.2836, 23.9429, 21.1242, 19.7191, 17.9639, 25.3872, 23.1988, 20.2987],
       grad_fn=<IndexBackward0>)
tensor([ 0.7684, 22.7900,  2.1049,  0.8118,  0.5042, 22.8300,  5.4673,  0.8133,
         0.5051, 28.9870,  4.3086,  1.6618,  0.5051, 21.5700,  5.1656,  0.7684])

        Epoch 0014 | Training loss 17.502306 | Training R2 0.203115 | Validation loss 19.610004 | Validation R2 -0.150834
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([11.4615, 22.3707, 18.7303, 12.3394, 19.1679, 15.6442,  9.1946],
       grad_fn=<IndexBackward0>)
tensor([ 5.5479, 51.8750, 15.8080,  2.3393, 50.7150, 15.6200,  2.3116])

        Epoch 0015 | Training loss 18.001534 | Training R2 0.157006 | Validation loss 23.457544 | Validation R2 -0.646730
        Best loss 18.415304 | Best epoch 0006

100%|########################################| 672/672 [01:32<00:00,  7.30it/s]
tensor([26.0862, 36.4665, 34.4420, 31.6990], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0016 | Training loss 17.815872 | Training R2 0.174305 | Validation loss 16.533590 | Validation R2 0.181928
        Best loss 16.533590 | Best epoch 0016

100%|########################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([20.8729, 27.1115, 26.6857, 26.2577, 25.8270, 24.5116, 29.1832, 27.9320,
        26.6842, 31.0547, 29.7846, 28.5277, 31.9418, 30.2244, 33.5438, 31.7833,
        35.0980, 33.2931, 36.6418, 34.7919, 38.0724, 36.1795, 39.4280, 37.4934,
        40.6823, 38.7079, 41.8330, 39.8208, 42.9237, 40.8747],
       grad_fn=<IndexBackward0>)
tensor([38.1730, 32.4920, 24.8420, 20.1090, 16.9610, 11.5390, 42.3870, 24.3350,
        16.9860, 47.3100, 27.9650, 19.6630, 34.2530, 20.9790, 35.0450, 21.5240,
        35.5990, 21.8790, 36.1540, 22.2220, 36.2560, 22.3030, 36.3190, 22.3450,
        36.2250, 22.2940, 36.0400, 22.1840, 35.9840, 22.1450])

        Epoch 0017 | Training loss 16.692785 | Training R2 0.275125 | Validation loss 17.948978 | Validation R2 0.035867
        Best loss 16.533590 | Best epoch 0016

100%|########################################| 672/672 [01:41<00:00,  6.63it/s]
tensor([11.4724, 18.8804, 17.5307, 16.9688, 16.3923, 14.5437, 18.8537, 17.8257,
        16.2227, 20.4424, 17.4939, 21.3679, 18.5040, 22.2148, 19.3835, 23.0034,
        20.1774, 23.7119, 20.8788, 24.3830, 21.5363, 25.0216, 22.1581],
       grad_fn=<IndexBackward0>)
tensor([21.3340, 19.2610, 14.4950, 11.2260,  8.9585,  5.3881, 18.6970, 12.5000,
         8.2546, 26.5910, 10.1260, 28.1980, 11.3250, 29.3320, 12.1280, 30.0900,
        12.6640, 30.4370, 12.9750, 30.7340, 13.1890, 30.9350, 13.3310])

        Epoch 0018 | Training loss 16.666876 | Training R2 0.277374 | Validation loss 15.139571 | Validation R2 0.314063
        Best loss 15.139571 | Best epoch 0018

100%|########################################| 672/672 [01:49<00:00,  6.11it/s]
tensor([ 9.6680, 15.9835,  6.9571, 18.1178, 13.7828], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0019 | Training loss 14.477341 | Training R2 0.454766 | Validation loss 13.607776 | Validation R2 0.445844
        Best loss 13.607776 | Best epoch 0019

100%|########################################| 672/672 [02:03<00:00,  5.43it/s]
tensor([ 9.4686, 38.3644, 12.2687, 11.5118,  9.2951], grad_fn=<IndexBackward0>)
tensor([ 2.7853, 66.9550,  2.7495,  2.3342,  2.7853])

        Epoch 0020 | Training loss 14.510922 | Training R2 0.452234 | Validation loss 16.810085 | Validation R2 0.154337
        Best loss 13.607776 | Best epoch 0019

100%|########################################| 672/672 [02:24<00:00,  4.64it/s]
tensor([ 8.5368, 33.8088, 18.8426,  7.7205, 27.9494, 14.5820,  7.0804, 27.8945,
        15.7736,  7.0733, 27.7991, 14.5482,  7.1518, 27.5038, 15.6676,  7.2093,
        27.8395, 15.8780,  7.2429, 27.8744, 15.9120,  7.2845, 27.1735, 14.3810,
         7.5503,  7.2736, 27.7247, 15.8215,  7.3511, 27.2426,  7.5329, 27.9717,
        16.0528,  7.4791], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900, 51.6110, 17.8000,  2.9402,
        52.2210, 18.0080,  2.9745, 52.2510, 18.0190,  2.9764, 50.5100, 15.1680,
         3.3052,  2.8777, 51.7310, 17.8380,  2.9464, 50.4840,  2.8761, 51.7290,
        17.8370,  2.9463])

        Epoch 0021 | Training loss 11.205886 | Training R2 0.673339 | Validation loss 10.361195 | Validation R2 0.678725
        Best loss 10.361195 | Best epoch 0021
```

```
100%|########################################| 672/672 [02:36<00:00,  4.28it/s]
tensor([ 7.2399, 32.7656, 15.4638,  8.0082,  6.0111,  5.5762, 17.2878,  7.8308,
         5.4720, 15.2764,  7.6041,  5.4436,  5.2924], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0022 | Training loss 9.869438 | Training R2 0.746610 | Validation loss 9.603258 | Validation R2 0.724009
        Best loss 9.603258 | Best epoch 0022

100%|########################################| 672/672 [02:32<00:00,  4.39it/s]
tensor([15.8579, 50.2009, 26.6418, 14.6086, 46.3771, 24.7828, 14.7037, 46.6151,
        14.9483, 46.6064, 25.1501, 15.1815, 46.7140, 25.3345, 15.4388, 46.7163,
        25.5262, 15.7424, 47.2646, 25.5042, 15.9307, 47.3325, 25.6759, 16.1516,
        25.6520, 16.3157, 47.7276, 26.3268, 16.6276, 48.0307, 26.6325],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0023 | Training loss 8.880115 | Training R2 0.794864 | Validation loss 7.997626 | Validation R2 0.808583
        Best loss 7.997626 | Best epoch 0023

100%|########################################| 672/672 [02:30<00:00,  4.48it/s]
tensor([17.2749, 69.2989, 34.9108, 18.0886, 29.8557, 17.5402, 65.0494, 31.9385,
        17.1078], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317])

        Epoch 0024 | Training loss 7.985860 | Training R2 0.834099 | Validation loss 8.102264 | Validation R2 0.803542
        Best loss 7.997626 | Best epoch 0023

100%|########################################| 672/672 [02:29<00:00,  4.49it/s]
tensor([11.3186, 17.6525,  7.2354,  5.7471, 42.5767, 15.1930,  9.6660,  6.2997,
         5.1429, 14.7872,  5.7812,  4.6024], grad_fn=<IndexBackward0>)
tensor([17.2550, 16.6050,  5.5696,  2.1836, 53.8670, 17.2450, 10.7980,  5.7840,
         2.2677, 17.4680,  5.8590,  2.2971])

        Epoch 0025 | Training loss 8.279782 | Training R2 0.821662 | Validation loss 9.688253 | Validation R2 0.719102
        Best loss 7.997626 | Best epoch 0023

100%|########################################| 672/672 [02:44<00:00,  4.09it/s]
tensor([15.5552, 21.2986,  8.9259, 19.4323,  8.8088, 49.8646, 19.4493,  8.6966,
        19.4075,  8.7305, 50.9847, 17.1765,  8.5072, 19.3949,  8.6471, 19.4621,
         8.3514, 19.4284,  8.7043,  7.9715, 19.3271,  7.7307, 19.0096,  7.5651,
        31.6473, 13.4038,  7.8101, 21.1455], grad_fn=<IndexBackward0>)
tensor([23.5920, 20.2570,  2.7573, 21.0380,  2.8637, 70.1770, 21.0260,  2.8620,
        21.0260,  2.8620, 70.1760, 18.0350,  2.8620, 21.0280,  2.8623, 21.0310,
         2.8627, 21.0320,  4.5357,  2.8628, 21.0320,  2.8627, 20.7940,  2.8304,
        37.6000, 12.7810,  2.7564, 23.5920])

        Epoch 0026 | Training loss 6.741351 | Training R2 0.881778 | Validation loss 6.505997 | Validation R2 0.873327
        Best loss 6.505997 | Best epoch 0026

100%|########################################| 672/672 [02:48<00:00,  3.99it/s]
tensor([ 6.7332, 80.9639, 29.2949, 11.5219,  8.3984, 20.1279,  7.6323, 57.2668,
        22.6112,  8.8510,  6.5061, 63.7430,  5.7285], grad_fn=<IndexBackward0>)
tensor([ 6.1430, 77.5480, 24.0970,  7.7805,  2.9525, 17.9790,  3.0428, 55.8410,
        21.1480,  6.8284,  3.0454, 63.6220,  2.9330])

        Epoch 0027 | Training loss 7.444011 | Training R2 0.855848 | Validation loss 8.489068 | Validation R2 0.784336
        Best loss 6.505997 | Best epoch 0026

100%|########################################| 672/672 [02:47<00:00,  4.01it/s]
tensor([ 7.7094, 43.7068, 36.5667, 25.8860, 12.6556,  7.2692,  4.5190,  3.7489,
        36.6624, 10.6850,  4.4337,  3.8561, 36.7842, 10.8842,  4.6113,  3.9674],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385])

        Epoch 0028 | Training loss 6.370688 | Training R2 0.894421 | Validation loss 5.628891 | Validation R2 0.905179
        Best loss 5.628891 | Best epoch 0028

100%|########################################| 672/672 [02:59<00:00,  3.75it/s]
tensor([ 3.2122, 45.6662, 11.4265,  2.6867], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0029 | Training loss 6.405765 | Training R2 0.893255 | Validation loss 6.673342 | Validation R2 0.866726
        Best loss 5.628891 | Best epoch 0028

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 2 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([2.2012, 4.3401, 4.5154, 4.6905, 4.8404, 7.3129, 9.4333, 9.6325, 9.8317],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0001 | Training loss 24.396061 | Training R2 -0.611271 | Validation loss 29.565437 | Validation R2 -1.135200
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.60it/s]
tensor([ 4.5868,  7.7243,  7.7393,  7.7542,  7.7692,  7.8141, 10.7971, 10.8420,
        10.8870, 13.8658, 13.9107, 13.9557, 16.8932, 16.9082, 16.9831, 19.9356,
        20.0105, 22.9630, 23.0379, 26.0379, 28.9479, 29.0378, 31.9629, 32.0378,
        34.8668, 34.9417, 37.7557, 37.8606], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590, 15.2690, 43.9280, 15.2390, 35.5910, 15.2300,
        34.7690, 14.8850, 42.5860, 12.5700])

        Epoch 0002 | Training loss 25.662014 | Training R2 -0.782833 | Validation loss 33.517918 | Validation R2 -1.744252
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([5.6275, 8.8024, 8.7686], grad_fn=<IndexBackward0>)
tensor([ 2.9348, 49.9870,  2.9348])

        Epoch 0003 | Training loss 24.307240 | Training R2 -0.599560 | Validation loss 31.725683 | Validation R2 -1.458623
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 7.0766, 10.0451,  9.7717,  9.5309,  9.2409, 11.8985, 11.5903, 11.2770,
        11.0037], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197])

        Epoch 0004 | Training loss 19.475636 | Training R2 -0.026863 | Validation loss 22.108311 | Validation R2 -0.193936
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([15.8276, 23.3258, 22.6143], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0005 | Training loss 20.458645 | Training R2 -0.133138 | Validation loss 24.160664 | Validation R2 -0.425895
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 9.2572, 13.8954, 12.9740], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0006 | Training loss 17.644037 | Training R2 0.157199 | Validation loss 18.924053 | Validation R2 0.125221
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([ 6.5554, 14.4303, 14.2323, 14.0333, 13.2285, 12.6145, 11.7806, 11.1425],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0007 | Training loss 17.723608 | Training R2 0.149580 | Validation loss 19.722084 | Validation R2 0.049886
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([17.9146, 28.9038, 27.0520, 23.5514, 30.4003, 28.1080, 23.7917, 29.1836,
        26.5059, 21.4689, 25.4389, 22.4455, 17.6895, 16.8178, 19.2722],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775, 17.6690])

        Epoch 0008 | Training loss 16.884079 | Training R2 0.228237 | Validation loss 18.234676 | Validation R2 0.187794
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([17.3961, 35.1640, 32.7303], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0009 | Training loss 17.305775 | Training R2 0.189205 | Validation loss 20.149847 | Validation R2 0.008224
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
```

```
tensor([ 0.9194,  2.6580,  2.2602,  1.8612,  1.4610, -0.2532, -1.1996, -1.9260,
        -2.2793], grad_fn=<IndexBackward0>)
tensor([0.3554, 5.3208, 4.0322, 3.2185, 2.6321, 1.2520, 0.7242, 0.3492, 0.2020])

        Epoch 0010 | Training loss 16.073269 | Training R2 0.300581 | Validation loss 18.079575 | Validation R2 0.201553
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([21.2469, 44.4680, 39.3766, 29.7086, 36.6719, 24.5128],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441])

        Epoch 0011 | Training loss 16.631989 | Training R2 0.251111 | Validation loss 19.968565 | Validation R2 0.025990
        Best loss 18.079575 | Best epoch 0010

 31%|###########7                            | 209/672 [00:28<00:59,  7.82it/s] 31%|###########7                            | 209/672 [00:29<01:05,  7.06it/s]
Traceback (most recent call last):
  File "/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py", line 94, in <module>
    loss.backward()
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/_tensor.py", line 363, in backward
    torch.autograd.backward(self, gradient, retain_graph, create_graph, inputs=inputs)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/autograd/__init__.py", line 173, in backward
    Variable._execution_engine.run_backward(  # Calls into the C++ engine to run the backward pass
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torch/autograd/function.py", line 253, in apply
    return user_fn(self, *args)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/adjoint.py", line 126, in backward
    aug_state = odeint(
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/odeint.py", line 77, in odeint
    solution = solver.integrate(t)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/solvers.py", line 30, in integrate
    solution[i] = self._advance(t[i])
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/rk_common.py", line 194, in _advance
    self.rk_state = self._adaptive_step(self.rk_state)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/rk_common.py", line 255, in _adaptive_step
    y1, f1, y1_error, k = _runge_kutta_step(self.func, y0, f0, t0, dt, t1, tableau=self.tableau)
  File "/Users/rishabhgoel/opt/anaconda3/lib/python3.9/site-packages/torchdiffeq/_impl/rk_common.py", line 75, in _runge_kutta_step
    yi = y0 + torch.sum(k[..., :i + 1] * (beta_i * dt), dim=-1).view_as(f0)
KeyboardInterrupt

(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % sh /Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run.sh
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 1 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 0.8659,  3.9961,  4.3409,  6.9639,  7.3083,  9.9335, 10.2554, 12.8904,
        13.2394], grad_fn=<IndexBackward0>)
tensor([ 2.9329, 18.1390,  2.8114, 19.1060,  2.9618, 16.6620,  2.9542, 19.3020,
         2.9922])

        Epoch 0001 | Training loss 24.626810 | Training R2 -0.641895 | Validation loss 30.045382 | Validation R2 -1.205085
        Best loss 30.045382 | Best epoch 0001

100%|########################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([4.6608, 9.5966, 9.7043, 9.7966], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0002 | Training loss 25.603544 | Training R2 -0.774718 | Validation loss 33.331497 | Validation R2 -1.713811
        Best loss 30.045382 | Best epoch 0001

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([ 6.3645, 10.0221, 10.0173, 10.0124], grad_fn=<IndexBackward0>)
tensor([ 2.0678, 51.9320, 15.5760,  5.7433])

        Epoch 0003 | Training loss 24.660084 | Training R2 -0.646335 | Validation loss 32.338074 | Validation R2 -1.554455
        Best loss 30.045382 | Best epoch 0001

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([ 7.5779, 10.7315, 10.5503, 10.3672], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.553848 | Training R2 -0.377116 | Validation loss 29.115191 | Validation R2 -1.070662
        Best loss 29.115191 | Best epoch 0004

100%|########################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([  9.4674,  12.8985,  12.3135,  11.0211,  14.3869,  13.7451,  12.2600,
         12.0065,  15.4448,  14.5974,  12.6249,  16.0483,  14.8118,  12.8713,
         16.2488,  15.8254,  12.6046,  15.9981,  14.5864,  11.8602,  15.3394,
         13.7693,  10.6944,  14.2434,  12.4934,   8.9465,  11.1621,   8.7467,
          6.5018,   8.8216,   6.4287,   3.5933,   5.7097,  -0.2928,   1.9313,
         -1.2142,  -4.9775,  -2.8409,  -6.3531, -10.4847,  -8.4183, -12.7798],
       grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568, 46.7250, 14.1790,  2.9953, 45.9950, 15.9060,
         2.9515, 45.8260, 15.7550,  2.9235, 46.3120, 16.0030,  2.9695, 46.4360,
        16.0330,  2.9750, 20.4610,  7.2470,  2.9262, 21.0770,  8.4980,  3.0144,
        20.5900,  2.9448, 20.6570,  8.3285,  2.9543, 20.5540,  8.2870,  2.9396,
        20.8050,  7.3688])

        Epoch 0005 | Training loss 24.629457 | Training R2 -0.642248 | Validation loss 31.366308 | Validation R2 -1.403238
        Best loss 29.115191 | Best epoch 0004

100%|########################################| 672/672 [01:31<00:00,  7.31it/s]
tensor([13.7938, 19.5351, 18.6905], grad_fn=<IndexBackward0>)
tensor([ 4.7871, 64.0820, 17.1420])

        Epoch 0006 | Training loss 19.594009 | Training R2 -0.039383 | Validation loss 22.387205 | Validation R2 -0.224249
        Best loss 22.387205 | Best epoch 0006

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([13.5974, 22.0083, 20.7167, 18.2056, 24.3761, 22.8267, 19.9298],
       grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978])

        Epoch 0007 | Training loss 21.656366 | Training R2 -0.269698 | Validation loss 25.866343 | Validation R2 -0.634331
        Best loss 22.387205 | Best epoch 0006

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([13.7767, 25.6110, 24.0869, 22.4042], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0008 | Training loss 19.849363 | Training R2 -0.066651 | Validation loss 22.911612 | Validation R2 -0.282275
        Best loss 22.387205 | Best epoch 0006

100%|########################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 6.9208, 16.1849, 15.8887, 15.5901, 14.3781, 13.4506, 12.1771, 10.2585,
        17.8604, 15.8144, 13.7238], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0009 | Training loss 19.794535 | Training R2 -0.060766 | Validation loss 23.148764 | Validation R2 -0.308957
        Best loss 22.387205 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([1.2596, 6.9738, 6.5930, 3.8516, 1.6130], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0010 | Training loss 18.974268 | Training R2 0.025326 | Validation loss 22.211109 | Validation R2 -0.205065
        Best loss 22.211109 | Best epoch 0010

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([18.5466, 29.4055, 26.8084, 21.3966, 29.5498, 26.6150, 21.1492, 28.1922,
        19.0624, 25.7390, 22.5225, 18.2763], grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558])

        Epoch 0011 | Training loss 17.096495 | Training R2 0.208696 | Validation loss 19.218676 | Validation R2 0.097771
        Best loss 19.218676 | Best epoch 0011

100%|########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([16.9351, 27.4040, 23.4701], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0012 | Training loss 16.428110 | Training R2 0.269358 | Validation loss 18.505262 | Validation R2 0.163511
        Best loss 18.505262 | Best epoch 0012

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([ 9.8728, 15.8824,  8.6026, 13.2544,  8.8886, 11.8249,  8.8372, 11.6379,
         9.4149,  9.0428, 12.0295,  9.4390,  9.0559, 12.1867,  9.2367,  8.8324,
        11.6683,  8.8186,  8.3951, 11.1735,  8.2062,  7.7652, 10.4920,  7.4185,
         6.9618,  9.3914,  6.4726,  6.0017,  8.6402], grad_fn=<IndexBackward0>)
tensor([15.8300, 13.0430,  1.2608, 15.9120,  1.2850, 11.0980,  1.0728, 11.0480,
         1.5299,  1.0679, 15.8290,  1.5298,  1.0679, 18.9520,  1.5296,  1.0678,
        15.8300,  1.5299,  1.0679, 15.8320,  1.5301,  1.0681, 15.8290,  1.5298,
         1.0679, 13.2230,  1.5298,  1.0679, 15.8300])

        Epoch 0013 | Training loss 15.320648 | Training R2 0.364547 | Validation loss 16.943941 | Validation R2 0.298708
        Best loss 16.943941 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([17.4992, 45.5948, 37.4352, 29.7296, 23.4574, 48.6114, 39.8724, 29.9042,
        23.3831, 32.9127, 26.3422, 22.5437, 35.1450, 29.7150, 26.0430, 23.3849],
       grad_fn=<IndexBackward0>)
```

```
tensor([ 8.4611, 79.6090, 23.5290,  8.0412,  3.2043, 82.3550, 24.5250,  7.1901,
         3.3400, 24.4960,  8.3718,  3.3360, 83.7380, 24.9400,  8.5236,  3.3965])

        Epoch 0014 | Training loss 14.304376 | Training R2 0.446055 | Validation loss 15.995668 | Validation R2 0.375008
        Best loss 15.995668 | Best epoch 0014

100%|##########################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([11.5216, 25.9536, 18.7742,  4.3684, 18.6990,  9.7573,  0.1605],
       grad_fn=<IndexBackward0>)
tensor([ 5.1847, 45.5960, 16.6720,  1.9627, 47.0920, 14.8530,  2.0373])

        Epoch 0015 | Training loss 13.305818 | Training R2 0.520695 | Validation loss 15.527839 | Validation R2 0.411032
        Best loss 15.527839 | Best epoch 0015

100%|##########################################| 672/672 [01:34<00:00,  7.14it/s]
tensor([28.4883, 51.7386, 40.8246, 30.6043], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0016 | Training loss 12.541238 | Training R2 0.574196 | Validation loss 15.046682 | Validation R2 0.446966
        Best loss 15.046682 | Best epoch 0016

100%|##########################################| 672/672 [01:35<00:00,  7.04it/s]
tensor([11.2521, 19.5203, 17.8567, 16.2123, 11.8429, 21.2629, 16.0014, 10.8984,
        19.3963, 14.2469, 10.8912, 16.2668, 11.1552, 15.9629, 11.2363, 16.5931,
        11.3656, 15.1527, 11.4783, 15.1492, 11.5536, 11.6942, 13.7656, 11.8604,
        13.7768, 11.9242, 13.7843, 11.9470], grad_fn=<IndexBackward0>)
tensor([19.5520, 16.4450, 14.1650, 12.2180,  7.8455, 26.0250, 16.5280, 10.6130,
        28.4130, 18.0610, 11.5980, 25.0280, 11.9480, 25.6030, 12.2220, 29.8010,
        12.1700, 25.3340, 12.0950, 25.5170, 12.1820, 12.4030, 19.4380, 12.4820,
        19.2730, 12.3760, 19.1570, 12.3010])

        Epoch 0017 | Training loss 11.577513 | Training R2 0.637123 | Validation loss 13.753815 | Validation R2 0.537921
        Best loss 13.753815 | Best epoch 0017

100%|##########################################| 672/672 [01:38<00:00,  6.81it/s]
tensor([10.4185, 26.7618, 24.2714, 21.8491, 19.4927, 13.1182, 24.9644, 19.7197,
        13.2779, 25.1034, 14.6586, 24.7988, 15.1336, 24.5942, 15.2684, 24.3810,
        15.0533, 24.1127, 14.4923, 23.7379, 14.2094, 23.2903, 14.0403],
       grad_fn=<IndexBackward0>)
tensor([21.3340, 19.2610, 14.4950, 11.2260,  8.9585,  5.3881, 18.6970, 12.5000,
         8.2546, 26.5910, 10.1260, 28.1980, 11.3250, 29.3320, 12.1280, 30.0980,
        12.6640, 30.4370, 12.9750, 30.7340, 13.1890, 30.9350, 13.3310])

        Epoch 0018 | Training loss 11.267155 | Training R2 0.656317 | Validation loss 12.282238 | Validation R2 0.631511
        Best loss 12.282238 | Best epoch 0018

100%|##########################################| 672/672 [02:00<00:00,  5.58it/s]
tensor([20.1693, 56.7647, 27.7908,  7.9118, 40.6580, 21.2197,  7.8559, 37.9466,
        21.1882,  8.0803, 38.2978, 21.6858,  9.4654], grad_fn=<IndexBackward0>)
tensor([21.5630, 60.7860, 21.2220,  3.9105, 61.5820, 21.8290,  4.0223, 60.9380,
        21.6020,  3.9807, 62.4120, 22.1240,  4.0767])

        Epoch 0019 | Training loss 9.092960 | Training R2 0.776159 | Validation loss 10.566298 | Validation R2 0.727281
        Best loss 10.566298 | Best epoch 0019

100%|##########################################| 672/672 [02:19<00:00,  4.82it/s]
tensor([ 9.1025, 45.4023, 15.0747,  1.2969, 33.6044, 13.7062,  2.0902, 32.2529,
        15.8544,  3.1089, 32.0395, 14.4172], grad_fn=<IndexBackward0>)
tensor([ 4.9161, 42.0730,  5.4589, 60.7050, 39.7010,  5.1625,  0.1270, 38.5530,
         6.6617,  0.1233, 37.8370,  4.9161])

        Epoch 0020 | Training loss 8.390466 | Training R2 0.809409 | Validation loss 10.254351 | Validation R2 0.743146
        Best loss 10.254351 | Best epoch 0020

100%|##########################################| 672/672 [02:33<00:00,  4.38it/s]
tensor([ 2.7823, -0.7012, 16.7425,  0.1005, 19.9626,  5.2998,  1.0183, 21.2979,
         8.5926], grad_fn=<IndexBackward0>)
tensor([ 5.8156,  0.8816, 16.1310,  0.8871, 19.8420,  3.7824,  0.8870, 20.1590,
         5.8156])

        Epoch 0021 | Training loss 7.370078 | Training R2 0.852947 | Validation loss 8.416509 | Validation R2 0.826965
        Best loss 8.416509 | Best epoch 0021

100%|##########################################| 672/672 [02:37<00:00,  4.27it/s]
tensor([ 7.6921, 42.0318, 11.1803,  2.1829,  0.5237,  0.5580, 17.6342,  3.8294,
         1.1199, 14.8636,  4.2910,  1.8874,  1.7715], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0022 | Training loss 6.769789 | Training R2 0.875926 | Validation loss 6.859765 | Validation R2 0.885055
        Best loss 6.859765 | Best epoch 0022

100%|##########################################| 672/672 [02:52<00:00,  3.91it/s]
tensor([11.5659, 52.0529, 15.9928,  4.2202, 45.0372, 15.4286,  4.4164, 43.9275,
         4.6320, 43.8827, 15.6865,  4.8887, 43.6431, 15.4863,  4.8999, 43.0473,
        15.1669,  4.7864, 41.8940, 14.7135,  4.8360,  6.5062,  4.7693, 54.8776,
         8.0003], grad_fn=<IndexBackward0>)
tensor([10.1490, 53.5670, 17.9020,  3.4087, 56.5400, 19.1720,  3.6506, 55.8710,
         3.6166, 56.8020, 19.0610,  3.6296, 56.8930, 19.0660,  3.6305, 55.6130,
        18.9050,  3.5998, 54.6240, 18.5710,  3.5362,  7.7903,  3.6241, 73.1600,
        10.1490])

        Epoch 0023 | Training loss 6.361078 | Training R2 0.890455 | Validation loss 6.279366 | Validation R2 0.903683
        Best loss 6.279366 | Best epoch 0023

100%|##########################################| 672/672 [02:51<00:00,  3.92it/s]
tensor([14.5146, 54.0734, 18.1540,  7.6142, 48.1451, 18.0857],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])

        Epoch 0024 | Training loss 6.199807 | Training R2 0.895940 | Validation loss 6.439827 | Validation R2 0.898698
        Best loss 6.279366 | Best epoch 0023

100%|##########################################| 672/672 [02:51<00:00,  3.92it/s]
tensor([10.2017, 18.5346,  7.6956,  5.7872, 45.1905, 18.6995, 12.8322,  8.4170,
         6.2132, 19.3536,  8.3681,  6.0190], grad_fn=<IndexBackward0>)
tensor([17.2550, 16.6050,  5.5696,  2.1836, 53.8670, 17.2450, 10.7980,  5.7840,
         2.2677, 17.4680,  5.8590,  2.2971])

        Epoch 0025 | Training loss 6.253183 | Training R2 0.894140 | Validation loss 6.411789 | Validation R2 0.899578
        Best loss 6.279366 | Best epoch 0023

100%|##########################################| 672/672 [02:45<00:00,  4.05it/s]
tensor([ 8.6411, 49.0276, 13.4753,  3.0070, 44.4376,  3.0360, 15.4121,  3.5914,
         2.9362, 15.4485,  2.8476, 18.0857,  3.8612,  2.7151, 15.4052,  4.9666,
         2.6273,  5.8230,  2.6753,  2.4607,  5.5406,  2.4344,  5.3797,  2.2320,
         4.8223], grad_fn=<IndexBackward0>)
tensor([ 7.7458, 46.1910, 15.8890,  2.9155, 46.8330,  2.9904, 18.0300,  5.5715,
         2.9028, 17.7490,  2.8574, 19.8480,  6.1265,  2.8016, 17.3840,  6.9723,
         2.7986,  7.9412,  3.1875,  2.7979,  7.8285,  2.7581,  7.8213,  2.7556,
         7.7458])

        Epoch 0026 | Training loss 5.956546 | Training R2 0.903945 | Validation loss 5.635359 | Validation R2 0.922427
        Best loss 5.635359 | Best epoch 0026

100%|##########################################| 672/672 [02:50<00:00,  3.94it/s]
tensor([ 4.2635, 45.8121, 11.2596,  1.9525,  0.8344, 44.7441, 12.2073,  2.7300,
         1.7247, 47.7349, 14.0866,  3.9717,  2.5308, 47.3887, 14.7678,  5.1951,
         3.2662], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105])

        Epoch 0027 | Training loss 7.578074 | Training R2 0.844530 | Validation loss 9.629846 | Validation R2 0.773479
        Best loss 5.635359 | Best epoch 0026

100%|##########################################| 672/672 [02:50<00:00,  3.95it/s]
tensor([ 8.8489, 19.4815, 12.3748, 31.3114, 21.7804], grad_fn=<IndexBackward0>)
tensor([18.2020, 14.6790,  8.2383, 35.7260, 18.2020])

        Epoch 0028 | Training loss 6.583239 | Training R2 0.882670 | Validation loss 6.253600 | Validation R2 0.904472
        Best loss 5.635359 | Best epoch 0026

100%|##########################################| 672/672 [02:49<00:00,  3.96it/s]
tensor([ 5.0181, 44.7492, 10.8638,  2.3139], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0029 | Training loss 6.611257 | Training R2 0.881669 | Validation loss 7.944351 | Validation R2 0.845835
        Best loss 5.635359 | Best epoch 0026

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 2 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################| 672/672 [01:33<00:00,  7.21it/s]
tensor([2.2012, 4.3401, 4.5154, 4.6905, 4.8404, 7.3129, 9.4333, 9.6325, 9.8317],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0001 | Training loss 24.396061 | Training R2 -0.611271 | Validation loss 29.565437 | Validation R2 -1.135200
        Best loss 29.565437 | Best epoch 0001
```

```
100%|########################################| 672/672 [01:31<00:00,  7.36it/s]
tensor([ 4.5868,  7.7243,  7.7393,  7.7542,  7.7692,  7.8141, 10.7971, 10.8420,
        10.8870, 13.8658, 13.9107, 13.9557, 16.8932, 16.9082, 16.9831, 19.9356,
        20.0105, 22.9630, 23.0379, 26.0379, 28.9479, 29.0378, 31.9629, 32.0378,
        34.8668, 34.9417, 37.7557, 37.8606], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590, 15.2690, 43.9280, 15.2390, 35.5910, 15.2300,
        34.7690, 14.8850, 42.5860, 12.5700])

        Epoch 0002 | Training loss 25.662014 | Training R2 -0.782833 | Validation loss 33.517918 | Validation R2 -1.744252
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:34<00:00,  7.10it/s]
tensor([5.6275, 8.8024, 8.7686], grad_fn=<IndexBackward0>)
tensor([ 2.9348, 49.9070,  2.9348])

        Epoch 0003 | Training loss 24.307240 | Training R2 -0.599560 | Validation loss 31.725683 | Validation R2 -1.458623
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:33<00:00,  7.18it/s]
tensor([ 7.0766, 10.0451,  9.7717,  9.5309,  9.2409, 11.8985, 11.5903, 11.2770,
        11.0037], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197])

        Epoch 0004 | Training loss 19.475636 | Training R2 -0.026863 | Validation loss 22.108311 | Validation R2 -0.193936
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:35<00:00,  7.01it/s]
tensor([15.8276, 23.3258, 22.6143], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0005 | Training loss 20.458645 | Training R2 -0.133138 | Validation loss 24.160664 | Validation R2 -0.425895
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([ 9.2572, 13.8954, 12.9740], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0006 | Training loss 17.644037 | Training R2 0.157199 | Validation loss 18.924053 | Validation R2 0.125221
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:33<00:00,  7.18it/s]
tensor([ 6.5554, 14.4303, 14.2323, 14.0333, 13.2285, 12.6145, 11.7806, 11.1425],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0007 | Training loss 17.723608 | Training R2 0.149580 | Validation loss 19.722084 | Validation R2 0.049886
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:32<00:00,  7.24it/s]
tensor([17.9146, 28.9038, 27.0520, 23.5514, 30.4003, 28.1080, 23.7917, 29.1836,
        26.5059, 21.4689, 25.4389, 22.4455, 17.6895, 16.8178, 19.2722],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775, 17.6690])

        Epoch 0008 | Training loss 16.884079 | Training R2 0.228237 | Validation loss 18.234676 | Validation R2 0.187794
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:35<00:00,  7.07it/s]
tensor([17.3961, 35.1640, 32.7303], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0009 | Training loss 17.305775 | Training R2 0.189205 | Validation loss 20.149847 | Validation R2 0.008224
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:35<00:00,  7.05it/s]
tensor([ 0.9194,  2.6580,  2.2602,  1.8612,  1.4610, -0.2532, -1.1996, -1.9260,
        -2.2793], grad_fn=<IndexBackward0>)
tensor([0.3554, 5.3208, 4.0322, 3.2185, 2.6321, 1.2520, 0.7242, 0.3492, 0.2020])

        Epoch 0010 | Training loss 16.073269 | Training R2 0.300581 | Validation loss 18.079575 | Validation R2 0.201553
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:33<00:00,  7.18it/s]
tensor([21.2469, 44.4680, 39.3766, 29.7086, 36.6719, 24.5128],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441])

        Epoch 0011 | Training loss 16.631989 | Training R2 0.251111 | Validation loss 19.968565 | Validation R2 0.025990
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:31<00:00,  7.37it/s]
tensor([-0.2112,  9.6766,  8.9151,  3.7237,  1.2923], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0012 | Training loss 16.117798 | Training R2 0.296700 | Validation loss 19.308783 | Validation R2 0.089291
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([ 8.1193, 28.2361, 13.4984], grad_fn=<IndexBackward0>)
tensor([ 2.9348, 49.9070,  2.9348])

        Epoch 0013 | Training loss 15.069706 | Training R2 0.385193 | Validation loss 17.587860 | Validation R2 0.244393
        Best loss 17.587860 | Best epoch 0013

100%|########################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([28.5283, 47.7753, 46.5215, 45.2703, 44.0218, 39.0541, 35.3557, 30.4602,
        26.8148, 23.1959, 40.9320, 28.8364, 19.7065, 14.5983],
       grad_fn=<IndexBackward0>)
tensor([50.4930, 47.4530, 35.8760, 28.7780, 23.7390, 11.8000,  7.0637,  3.5658,
         2.1356,  1.2790, 48.6290, 12.1880,  3.6833,  1.3211])

        Epoch 0014 | Training loss 13.840353 | Training R2 0.481411 | Validation loss 15.888102 | Validation R2 0.383385
        Best loss 15.888102 | Best epoch 0014

100%|########################################| 672/672 [01:31<00:00,  7.38it/s]
tensor([19.5747, 57.5473, 43.1012, 17.4868, 42.4553, 25.7603, 14.2486, 30.5511,
        15.0762, 24.2108, 19.7464], grad_fn=<IndexBackward0>)
tensor([17.5830, 71.0850, 22.2940,  2.9600, 49.2230, 14.1200,  2.9876, 52.3580,
         3.1778, 44.7320, 17.5830])

        Epoch 0015 | Training loss 13.451623 | Training R2 0.510133 | Validation loss 15.478939 | Validation R2 0.414735
        Best loss 15.478939 | Best epoch 0015

100%|########################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([15.3390, 40.8979, 27.4991,  6.8975, 27.3409, 16.6550],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0016 | Training loss 12.981250 | Training R2 0.543793 | Validation loss 14.996788 | Validation R2 0.450628
        Best loss 14.996788 | Best epoch 0016

100%|########################################| 672/672 [01:31<00:00,  7.36it/s]
tensor([20.6242, 87.1770, 56.6517], grad_fn=<IndexBackward0>)
tensor([12.6410, 93.0030, 31.3750])

        Epoch 0017 | Training loss 12.344368 | Training R2 0.587459 | Validation loss 14.402932 | Validation R2 0.493276
        Best loss 14.402932 | Best epoch 0017

100%|########################################| 672/672 [01:31<00:00,  7.31it/s]
tensor([ 5.8743, 33.4952, 14.7101,  2.2171, -1.6118, -3.1793, 19.0814,  7.9290,
         2.0781, -3.3863,  6.3008,  0.5193, -5.0548], grad_fn=<IndexBackward0>)
tensor([ 3.4332, 50.3360, 16.1560,  3.8901,  1.9088,  1.3372, 50.8530, 13.6880,
         5.6217,  1.3536, 19.2430,  5.5348,  1.1154])

        Epoch 0018 | Training loss 11.731128 | Training R2 0.627429 | Validation loss 13.635745 | Validation R2 0.545820
        Best loss 13.635745 | Best epoch 0018

100%|########################################| 672/672 [01:32<00:00,  7.24it/s]
tensor([ 9.1925, 60.4866, 25.4927,  2.9691, 22.6411,  3.5867, 18.8998,  2.9576,
        16.7243,  2.9704], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0019 | Training loss 11.256901 | Training R2 0.656943 | Validation loss 13.020782 | Validation R2 0.585863
        Best loss 13.020782 | Best epoch 0019

100%|########################################| 672/672 [01:33<00:00,  7.16it/s]
tensor([13.8924, 49.3759, 17.0867,  2.1433, 32.8296, 15.3211,  1.6264],
       grad_fn=<IndexBackward0>)
tensor([14.0340, 52.5400, 13.3690,  1.8996, 54.8650, 14.0150,  1.9913])

        Epoch 0020 | Training loss 10.266763 | Training R2 0.714638 | Validation loss 12.052997 | Validation R2 0.645138
        Best loss 12.052997 | Best epoch 0020

100%|########################################| 672/672 [01:36<00:00,  6.98it/s]
tensor([ 1.2734, 12.3216, -0.0398,  9.7799,  0.8759], grad_fn=<IndexBackward0>)
tensor([0.1803, 6.8826, 0.1879, 5.1060, 0.1803])

        Epoch 0021 | Training loss 9.368041 | Training R2 0.762411 | Validation loss 10.987734 | Validation R2 0.705092
        Best loss 10.987734 | Best epoch 0021

100%|########################################| 672/672 [01:38<00:00,  6.83it/s]
tensor([ 2.8928,  7.5500,  1.0634, -2.5524, 21.9355,  8.8222,  1.5529, -0.8570,
        -1.7677,  8.2143,  4.1006, -1.0089], grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625, 15.0820,  8.0548,  1.9640])

        Epoch 0022 | Training loss 8.574180 | Training R2 0.800972 | Validation loss 9.521894 | Validation R2 0.778529
        Best loss 9.521894 | Best epoch 0022

100%|########################################| 672/672 [01:43<00:00,  6.48it/s]
tensor([11.8306, 63.7298, 21.1029,  1.9694, 50.4705, 22.5680,  4.1765, 49.5880,
        23.2013, 11.2773,  6.1622], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])
```

```
        Epoch 0023 | Training loss 8.035305 | Training R2 0.825203 | Validation loss 9.607019 | Validation R2 0.774552
        Best loss 9.521894 | Best epoch 0022

100%|##########################################| 672/672 [01:59<00:00,  5.64it/s]
tensor([ 6.3880, 14.1343,  2.3735, 29.4463, 13.7770,  2.6396, 30.1243, 13.3924,
         2.9050, 30.8156, 13.5442,  3.0128, 30.5357, 13.4501],
       grad_fn=<IndexBackward0>)
tensor([ 9.8032,  9.6259,  0.6383, 43.8570,  9.7042,  0.6435, 44.0790,  9.7534,
         0.6467, 44.4320,  9.8362,  0.6522, 44.3840,  9.8032])

        Epoch 0024 | Training loss 7.263038 | Training R2 0.857188 | Validation loss 8.324299 | Validation R2 0.830736
        Best loss 8.324299 | Best epoch 0024

100%|##########################################| 672/672 [02:16<00:00,  4.91it/s]
tensor([26.6158, 57.6124], grad_fn=<IndexBackward0>)
tensor([47.8150, 46.0380])

        Epoch 0025 | Training loss 6.618134 | Training R2 0.881423 | Validation loss 6.747346 | Validation R2 0.888792
        Best loss 6.747346 | Best epoch 0025

100%|##########################################| 672/672 [02:25<00:00,  4.62it/s]
tensor([ 8.1440, 64.3160, 18.0991,  0.7626, 17.8471,  1.6511, 16.7843,  1.7408,
        16.2581,  1.1391], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0026 | Training loss 6.682505 | Training R2 0.879105 | Validation loss 6.442039 | Validation R2 0.898628
        Best loss 6.442039 | Best epoch 0026

100%|##########################################| 672/672 [02:29<00:00,  4.48it/s]
tensor([ 3.0113, 11.6365,  1.9527], grad_fn=<IndexBackward0>)
tensor([2.0948, 9.5297, 2.0948])

        Epoch 0027 | Training loss 6.799114 | Training R2 0.874849 | Validation loss 6.605771 | Validation R2 0.893410
        Best loss 6.442039 | Best epoch 0026

100%|##########################################| 672/672 [02:33<00:00,  4.39it/s]
tensor([10.0965, 64.9965, 18.0683,  2.7577, 49.3049, 19.3117,  7.8974,  5.1164],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018])

        Epoch 0028 | Training loss 7.477236 | Training R2 0.848640 | Validation loss 9.610397 | Validation R2 0.774393
        Best loss 6.442039 | Best epoch 0026

100%|##########################################| 672/672 [02:34<00:00,  4.36it/s]
tensor([ 6.7122, 47.8820, 13.4944,  2.2469], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0029 | Training loss 6.323672 | Training R2 0.891740 | Validation loss 5.862009 | Validation R2 0.916061
        Best loss 5.862009 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 3 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################| 672/672 [01:27<00:00,  7.66it/s]
tensor([ 2.1615,  4.8593,  5.0546,  5.4167,  7.8210,  8.3762, 10.8642, 11.1145,
        11.2536, 13.7084, 14.0987], grad_fn=<IndexBackward0>)
tensor([ 7.7458, 46.1910, 15.8890,  2.9155, 46.8330,  2.9904, 18.0300,  5.5715,
         2.9028, 17.7490,  2.8574])

        Epoch 0001 | Training loss 25.062193 | Training R2 -0.700463 | Validation loss 31.127050 | Validation R2 -1.366714
        Best loss 31.127050 | Best epoch 0001

100%|##########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([4.8389, 7.9815, 8.0795, 8.1939], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0002 | Training loss 25.686121 | Training R2 -0.786184 | Validation loss 33.511566 | Validation R2 -1.743212
        Best loss 31.127050 | Best epoch 0001

100%|##########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([10.7876, 14.7278, 14.7281, 14.7284, 14.7289, 14.7298, 14.7307, 14.7318,
        14.7326], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0003 | Training loss 24.546101 | Training R2 -0.631151 | Validation loss 32.111191 | Validation R2 -1.518737
        Best loss 31.127050 | Best epoch 0001

100%|##########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([3.3280, 8.1569], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0004 | Training loss 22.813705 | Training R2 -0.409032 | Validation loss 29.552938 | Validation R2 -1.133395
        Best loss 29.552938 | Best epoch 0004

100%|##########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([2.0743, 3.6892, 3.5648, 3.4382, 3.1781, 2.7698, 2.3375, 1.7664, 1.4013],
       grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0005 | Training loss 18.439297 | Training R2 0.079513 | Validation loss 20.436989 | Validation R2 -0.020243
        Best loss 20.436989 | Best epoch 0005

100%|##########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([14.8184, 21.9938, 21.1540, 19.1529, 25.6132, 24.3171, 21.8638, 28.2239,
        26.6049, 23.5441, 29.8066, 27.8578, 24.1761], grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781, 68.7910,
        23.4760,  4.5602, 68.2770, 23.3020,  4.5263])

        Epoch 0006 | Training loss 17.760878 | Training R2 0.146000 | Validation loss 19.276941 | Validation R2 0.092292
        Best loss 19.276941 | Best epoch 0006

100%|##########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([ 7.2685, 17.8126, 17.6222, 17.4313, 16.6626, 16.0806, 15.2971, 14.1049,
        19.7325, 18.0599, 16.3651], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0007 | Training loss 17.224669 | Training R2 0.196787 | Validation loss 18.606171 | Validation R2 0.154363
        Best loss 18.606171 | Best epoch 0007

100%|##########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([ 8.3480, 18.9609, 17.0796, 13.5076, 19.1425, 16.7568, 12.2467, 17.5037,
        15.0191,  9.3061, 14.1835, 11.0108], grad_fn=<IndexBackward0>)
tensor([ 4.9161, 42.0730,  5.4589, 60.7050, 39.7010,  5.1625,  0.1270, 38.5530,
         6.6617,  0.1233, 37.8370,  4.9161])

        Epoch 0008 | Training loss 16.808960 | Training R2 0.235089 | Validation loss 18.387007 | Validation R2 0.174167
        Best loss 18.387007 | Best epoch 0008

100%|##########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([ 5.5405, 18.0450, 15.2522, 13.2369, 12.8317, 18.4610, 14.6685, 11.4213,
        11.8837, 10.3732, 10.1442, 13.0661, 11.2028,  9.8967,  9.6595],
       grad_fn=<IndexBackward0>)
tensor([ 9.8083, 13.5140,  3.7950,  1.5319,  1.2778, 13.2800,  3.7295,  1.2557,
         3.7290,  1.5053,  1.2555, 13.1880,  3.7035,  1.4950,  1.2470])

        Epoch 0009 | Training loss 16.176075 | Training R2 0.291605 | Validation loss 17.658480 | Validation R2 0.238313
        Best loss 17.658480 | Best epoch 0009

100%|##########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 4.4795, 11.8215,  9.0239,  6.1657, 12.2526,  8.1955,  6.0050,  5.2888,
         5.0226], grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625])

        Epoch 0010 | Training loss 15.784349 | Training R2 0.325499 | Validation loss 17.559269 | Validation R2 0.246848
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.62it/s]
tensor([12.7334, 35.1197, 29.4521, 23.7096, 18.7326, 32.3226, 24.1075],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0011 | Training loss 19.306719 | Training R2 -0.009128 | Validation loss 25.415319 | Validation R2 -0.577833
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([32.0389, 42.7443, 41.9388, 41.1327, 39.5190, 37.9050, 47.3776, 44.0538,
        40.7275, 49.5277, 43.8861, 41.0659, 49.2414, 39.0088, 46.8657, 34.8696,
        42.4265, 29.7071, 36.3832, 27.1146, 31.6529, 26.3287, 30.2598, 25.4865],
       grad_fn=<IndexBackward0>)
tensor([58.5520, 41.9580, 32.6790, 27.1470, 20.1960, 15.4500, 55.2420, 32.3270,
        21.5820, 60.6230, 31.3470, 24.0360, 61.8120, 24.6620, 62.3610, 24.9130,
        62.5810, 25.0130, 62.4280, 24.9640, 62.3850, 24.9450, 62.3680, 24.9370])

        Epoch 0012 | Training loss 15.314219 | Training R2 0.365080 | Validation loss 18.021051 | Validation R2 0.206713
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.56it/s]
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```
tensor([ 0.5030,  2.0243,  1.2888,  0.5755,  0.0550, -1.1188, -1.4900, -1.7581,
        -1.9126, -2.0494, -1.1390, -1.4614, -1.5448, -1.7284, -1.9236],
       grad_fn=<IndexBackward0>)
tensor([0.1027, 4.3675, 3.3207, 2.6789, 2.2198, 1.1160, 0.6726, 0.3426, 0.2866,
        0.1245, 4.4427, 1.1442, 0.8164, 0.3513, 0.1277])

        Epoch 0013 | Training loss 14.627570 | Training R2 0.420740 | Validation loss 16.876558 | Validation R2 0.304275
        Best loss 16.876558 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 8.8011, 44.5529, 42.7156, 40.8827, 31.7829, 26.4018, 19.3116,  9.0496,
        38.4039, 23.2554, 15.9224, 11.0489, 20.7719, 15.0965, 11.2353, 18.4193,
        15.1102, 12.8798, 18.1327, 16.6533, 15.1084, 19.4565, 18.0770, 16.5790,
        18.9628], grad_fn=<IndexBackward0>)
tensor([ 4.2077, 59.4320, 46.9050, 38.1280, 14.2580,  7.9220,  3.6186,  1.1171,
        59.4890, 17.3990,  4.4157,  1.1207, 17.1950,  4.3640,  1.1075, 17.2810,
         4.3856,  1.1130, 16.8630,  5.2057,  1.0861, 16.8560,  4.2779,  1.0857,
         4.2077])

        Epoch 0014 | Training loss 13.552494 | Training R2 0.502758 | Validation loss 15.915753 | Validation R2 0.381237
        Best loss 15.915753 | Best epoch 0014

100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([ 4.4982, 21.3597,  5.1706], grad_fn=<IndexBackward0>)
tensor([ 4.6703, 20.6660,  3.8425])

        Epoch 0015 | Training loss 13.312044 | Training R2 0.520246 | Validation loss 15.572647 | Validation R2 0.407628
        Best loss 15.572647 | Best epoch 0015

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 5.1438,  8.7150,  8.2335, 17.3058, 10.0088,  9.1330, 17.2026, 10.6696,
        10.4114], grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462])

        Epoch 0016 | Training loss 12.642657 | Training R2 0.567281 | Validation loss 14.518663 | Validation R2 0.485100
        Best loss 14.518663 | Best epoch 0016

100%|########################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([ 8.6458, 39.9109, 19.5235,  1.5698, 25.5519, 13.4577,  2.6799],
       grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173])

        Epoch 0017 | Training loss 12.009523 | Training R2 0.609536 | Validation loss 13.955899 | Validation R2 0.524243
        Best loss 13.955899 | Best epoch 0017

100%|########################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([16.5268, 53.2245, 25.6311,  4.3723, 32.4923, 17.3056,  3.8944, 25.6408,
        15.9058,  4.0992], grad_fn=<IndexBackward0>)
tensor([12.3700, 69.3770, 19.4920,  2.1362, 68.1120, 16.1970,  2.1042, 46.9250,
        16.8400,  2.1878])

        Epoch 0018 | Training loss 11.491714 | Training R2 0.642481 | Validation loss 14.003984 | Validation R2 0.520958
        Best loss 13.955899 | Best epoch 0017

100%|########################################| 672/672 [01:31<00:00,  7.31it/s]
tensor([12.2880, 60.9434, 23.6948,  3.7652, 41.1423, 23.2139,  4.3050, 37.7644,
        21.6612, 10.9115,  4.7921, 33.1801, 17.9587,  9.4201,  4.5785],
       grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370, 62.9420, 16.8690,  6.5668,  3.3492])

        Epoch 0019 | Training loss 10.620493 | Training R2 0.694636 | Validation loss 12.171548 | Validation R2 0.638123
        Best loss 12.171548 | Best epoch 0019

100%|########################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([17.7791, 60.7902, 21.8121,  3.3622, 36.1535, 18.7518,  3.8016, 34.5173,
        18.5345,  3.7166], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4989, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0020 | Training loss 9.667159 | Training R2 0.746996 | Validation loss 11.243977 | Validation R2 0.691177
        Best loss 11.243977 | Best epoch 0020

100%|########################################| 672/672 [01:35<00:00,  7.06it/s]
tensor([ 6.4277, 43.8652, 10.8547,  0.8505], grad_fn=<IndexBackward0>)
tensor([ 1.7780, 53.9210, 16.2500,  5.2152])

        Epoch 0021 | Training loss 9.009152 | Training R2 0.780266 | Validation loss 9.978053 | Validation R2 0.756801
        Best loss 9.978053 | Best epoch 0021

100%|########################################| 672/672 [01:38<00:00,  6.82it/s]
tensor([ 7.1529, 44.6963, 12.5524,  2.6736, -0.6076, -1.8314, 12.8853,  3.2542,
         0.2715, -0.8585, 10.7207,  4.6728,  1.5571,  0.3938],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8804,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0022 | Training loss 8.104481 | Training R2 0.822180 | Validation loss 8.888013 | Validation R2 0.807035
        Best loss 8.888013 | Best epoch 0022

100%|########################################| 672/672 [01:44<00:00,  6.46it/s]
tensor([ 9.0191, 62.1389,  0.5210, -0.0926,  2.1431], grad_fn=<IndexBackward0>)
tensor([ 2.7853, 66.9550,  2.7495,  2.3342,  2.7853])

        Epoch 0023 | Training loss 8.010061 | Training R2 0.826300 | Validation loss 9.681182 | Validation R2 0.771057
        Best loss 8.888013 | Best epoch 0022

100%|########################################| 672/672 [01:56<00:00,  5.76it/s]
tensor([ 3.4122,  6.5380,  0.7621, -1.5433, 25.6093,  7.9584,  1.0656, -0.6848,
        -1.0974,  7.6864,  3.0400, -1.3328, 15.6097,  3.6924, -0.7531, -1.4187,
        17.5918,  4.1631, -0.1998, -1.6550, 11.6587, -1.1651, -2.1033, 22.8726,
         5.6306, -0.3096, -2.2767, 22.2590,  5.2173, -0.8715, -2.5756, 21.4615,
         3.5346, -1.2039, -2.7982, 20.7264,  1.8163, -2.2834],
       grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625, 15.0820,  8.0548,  1.9640, 29.0970,  9.7026,  3.2372,  2.0224,
        33.9450, 11.2970,  4.4089,  2.0129, 24.7420,  3.7684,  2.0126, 48.9190,
        15.4550,  5.1565,  2.0125, 48.9190, 15.4550,  5.1565,  2.0125, 48.9190,
        13.2120,  5.1565,  2.0125, 48.9190, 11.2950,  3.7684])

        Epoch 0024 | Training loss 7.332561 | Training R2 0.854441 | Validation loss 7.375947 | Validation R2 0.867106
        Best loss 7.375947 | Best epoch 0024

100%|########################################| 672/672 [02:15<00:00,  4.96it/s]
tensor([17.5115, 75.5686, 24.1151,  5.0300, 47.8906, 15.6807,  4.7381, 48.6322,
         3.4479, 40.0268, 15.2362], grad_fn=<IndexBackward0>)
tensor([17.5830, 71.0850, 22.2940,  2.9600, 49.2230, 14.1200,  2.9876, 52.3580,
         3.1778, 44.7320, 17.5830])

        Epoch 0025 | Training loss 8.509421 | Training R2 0.803967 | Validation loss 9.115965 | Validation R2 0.797010
        Best loss 7.375947 | Best epoch 0024

100%|########################################| 672/672 [02:22<00:00,  4.71it/s]
tensor([ 9.7489, 43.1830, 33.0272, 24.0184, 12.7075,  8.0704,  4.5794,  2.5688,
        37.6630, 14.1537,  6.5239,  4.7297, 40.0373, 15.7862,  7.8193,  6.2941,
        41.6687, 24.4670,  7.7723,  7.5809, 42.2466, 14.8588, 10.3533,  8.6096,
        42.5899, 18.5460, 11.0454,  9.2425, 43.5388, 17.5699, 11.5147,  9.8455,
        44.1187, 19.8935, 11.9677, 10.3997, 44.5415, 20.4890],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385,
        43.0630, 20.8330,  1.9210,  1.3667, 43.0860,  8.8969,  3.7979,  1.3674,
        42.5380, 12.3470,  3.7496,  1.3500, 42.9850, 10.5230,  3.7888,  1.3642,
        43.0840, 12.5050,  3.7977,  1.3674, 43.0840, 12.5050])

        Epoch 0026 | Training loss 7.642862 | Training R2 0.841860 | Validation loss 9.652371 | Validation R2 0.772418
        Best loss 7.375947 | Best epoch 0024

100%|########################################| 672/672 [02:25<00:00,  4.61it/s]
tensor([ 8.1295, 16.1995,  3.9024, 38.7570, 16.0048], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0027 | Training loss 6.217919 | Training R2 0.895331 | Validation loss 6.709231 | Validation R2 0.890045
        Best loss 6.709231 | Best epoch 0027

100%|########################################| 672/672 [02:29<00:00,  4.50it/s]
tensor([ 2.9591, 16.0822,  0.4870, 41.0720, 13.1148,  0.7645, 43.0557, 15.5036,
         2.9654,  1.1200, 14.4833,  3.8689,  1.5330, 17.2718,  4.1735,  2.0491,
         5.0674,  2.6229,  7.1752,  3.4310, 51.3981,  6.0681,  3.6774,  8.0776,
         4.6272, 41.4533,  7.2808,  4.7518], grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742, 43.9160, 13.4380,
         2.8234,  1.0649, 12.6990,  3.2428,  1.0064, 15.4190,  3.2397,  1.0054,
         3.3101,  1.0273,  4.8677,  1.0228, 53.4230,  3.3111,  1.0275,  4.8942,
         1.0283, 40.7690,  3.8721,  0.9887])

        Epoch 0028 | Training loss 6.206502 | Training R2 0.895715 | Validation loss 7.057861 | Validation R2 0.878321
        Best loss 6.709231 | Best epoch 0027

100%|########################################| 672/672 [02:31<00:00,  4.45it/s]
tensor([ 7.6626, 77.2475, 59.0601, 48.7603, 39.5699, 12.5270,  0.4892, -2.0569,
        -3.5056, 59.4931, 14.3282,  1.8468, -1.0112, 59.4113, 14.9668,  2.1448,
        -0.3603, 60.1407, 15.7482,  2.9394,  0.3238], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947, 73.8930, 26.4440, 10.0160,
         5.0069, 74.0470, 26.5260, 10.0480,  5.0226])

        Epoch 0029 | Training loss 5.844729 | Training R2 0.907518 | Validation loss 5.710489 | Validation R2 0.920344
        Best loss 5.710489 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
```

```
See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 4 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 2.8156,  6.4742,  6.6527,  6.8312,  6.9842, 10.4804, 10.6588],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0001 | Training loss 25.589478 | Training R2 -0.772768 | Validation loss 32.346756 | Validation R2 -1.555826
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([1.9038, 5.0573, 5.0673, 5.1375, 5.1977], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0002 | Training loss 25.551172 | Training R2 -0.767465 | Validation loss 33.349823 | Validation R2 -1.716795
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 5.6753,  9.1968,  9.1520,  9.1070,  9.0680, 12.3688, 12.3259, 12.2829,
        12.2460, 15.6801, 15.6373, 15.5945, 15.5579, 18.8876, 18.8448, 18.8021,
        18.7654, 22.0656, 22.0229, 21.9801, 21.9435, 25.1256, 25.0829, 25.0402,
        25.0036, 28.1739, 28.1312, 28.0886, 28.0520, 31.1455, 31.1029, 31.0603,
        31.0238, 34.1763, 34.1337, 34.0912, 34.0547, 37.1030, 37.0544, 37.0118,
        40.1939, 40.1514, 40.1089, 40.0725, 43.2250, 43.1825, 43.1401, 43.1036,
        46.1381, 46.0957, 46.0532, 46.0168, 48.9333, 48.8909, 48.8121, 51.7009,
        51.6585, 51.6222, 54.7601, 54.6392, 57.7422, 57.6999, 57.6637],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0003 | Training loss 25.064499 | Training R2 -0.700776 | Validation loss 33.287090 | Validation R2 -1.706584
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([11.9925, 16.1087, 15.6565, 14.7926, 18.7813, 18.1950, 17.1649],
       grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517])

        Epoch 0004 | Training loss 19.580549 | Training R2 -0.037956 | Validation loss 22.115347 | Validation R2 -0.194696
        Best loss 22.115347 | Best epoch 0004

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([11.7457, 16.1828, 15.2492], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0005 | Training loss 17.637089 | Training R2 0.157863 | Validation loss 18.753033 | Validation R2 0.140961
        Best loss 18.753033 | Best epoch 0005

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([18.9408, 25.6120, 24.2652, 21.7064, 27.7522, 26.0064, 22.9544, 28.8805,
        26.7267, 22.9661], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0006 | Training loss 17.212334 | Training R2 0.197937 | Validation loss 18.404135 | Validation R2 0.172628
        Best loss 18.404135 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 7.4809, 16.4973, 14.5521, 12.8453, 11.0989, 10.8038, 14.5344, 11.6942,
         9.5260,  9.1614], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530])

        Epoch 0007 | Training loss 18.241096 | Training R2 0.099195 | Validation loss 21.649376 | Validation R2 -0.144882
        Best loss 18.404135 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([21.2631, 37.7968, 34.6909, 28.8175, 35.9441, 28.1752, 40.1245, 34.2910,
        23.3075, 27.6585, 19.4856, 23.0779, 19.0806, 24.1141, 21.9171],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836, 23.7820,  3.2723, 61.1610, 20.1800])

        Epoch 0008 | Training loss 15.880821 | Training R2 0.317229 | Validation loss 17.267464 | Validation R2 0.271672
        Best loss 17.267464 | Best epoch 0008

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([29.5514, 33.9478, 33.5019, 33.0550, 31.7080, 36.2872, 34.6281, 32.9590,
        35.4917, 33.4942, 37.8418, 33.2047, 37.4423, 32.1499, 36.2251, 30.2793,
        34.2453, 27.6422, 31.5599, 24.2538, 28.0946, 21.8433, 24.2154],
       grad_fn=<IndexBackward0>)
tensor([66.9750, 34.8300, 30.4850, 27.1220, 19.3810, 59.4210, 39.4690, 28.2220,
        45.4640, 32.5130, 71.1690, 34.2430, 72.7160, 35.0360, 72.9860, 35.1970,
        73.1260, 35.2700, 73.7120, 35.5420, 73.9550, 35.6660, 66.9750])

        Epoch 0009 | Training loss 15.588125 | Training R2 0.342165 | Validation loss 17.531309 | Validation R2 0.249244
        Best loss 17.267464 | Best epoch 0008

100%|########################################| 672/672 [01:30<00:00,  7.47it/s]
tensor([22.3988, 44.0035, 38.3123, 27.5719, 42.2598, 33.7127, 17.9093, 31.7069,
        21.5951, 15.1084, 21.6086, 18.1968, 14.7075, 19.6320, 17.6338, 14.6714,
        18.9939, 17.1625, 14.7096, 18.3896, 16.8863, 14.2772, 17.6625, 16.0937,
        14.1760, 16.9282, 15.6259, 13.6606, 16.4278, 15.1709],
       grad_fn=<IndexBackward0>)
tensor([22.8850, 73.4140, 23.4880,  3.5482, 76.4500, 24.6180,  3.7189, 76.3100,
        24.5840,  3.7138, 76.0510, 21.1850,  3.7013, 75.8210, 24.4220,  3.6893,
        74.9130, 24.1510,  3.6483, 73.3630, 23.6320,  3.5700, 72.1350, 23.2310,
         3.5094, 70.4750, 19.6300,  3.4295, 70.9820, 22.8850])

        Epoch 0010 | Training loss 15.053199 | Training R2 0.386539 | Validation loss 16.905653 | Validation R2 0.301874
        Best loss 16.905653 | Best epoch 0010

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([18.1234, 47.1816, 39.9245], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0011 | Training loss 14.768456 | Training R2 0.409528 | Validation loss 16.615559 | Validation R2 0.325627
        Best loss 16.615559 | Best epoch 0011

100%|########################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([11.6720, 32.8382, 24.0419,  7.9924, 23.3818, 12.4458,  8.1120, 14.4407,
        11.5844,  8.4578], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0790,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225])

        Epoch 0012 | Training loss 14.076530 | Training R2 0.463561 | Validation loss 15.982780 | Validation R2 0.376014
        Best loss 15.982780 | Best epoch 0012

100%|########################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([15.4169, 37.7438, 26.4691,  7.0804, 27.0034, 15.1891],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0013 | Training loss 13.712152 | Training R2 0.490973 | Validation loss 15.644684 | Validation R2 0.402134
        Best loss 15.644684 | Best epoch 0013

100%|########################################| 672/672 [01:31<00:00,  7.37it/s]
tensor([12.0577, 36.3803, 23.6637, 11.4284,  3.9892, 24.7131, 13.2179,  7.2145,
         3.9259, 17.6060, 11.4485,  7.1599,  4.1087, 14.8795, 10.1405,  7.4436,
         5.7456, 12.6350, 10.5755,  8.8864,  7.3162, 13.0429, 11.6113,  9.6312,
         8.1763, 13.7002, 12.1540, 10.3492,  8.4799, 14.0624, 12.3707],
       grad_fn=<IndexBackward0>)
tensor([15.8670, 48.0290, 15.0320,  5.2611,  2.1393, 49.5140, 15.6140,  5.4648,
         2.2222, 49.5850, 15.6390,  5.4735,  2.2257, 49.6100, 15.6440,  5.4753,
         2.2264, 49.5890, 15.6410,  5.4740,  2.2259, 49.5930, 15.6410,  4.7118,
         2.2260, 49.5930, 15.6410,  5.4742,  2.2260, 50.3130, 15.8670])

        Epoch 0014 | Training loss 13.242213 | Training R2 0.525266 | Validation loss 15.322500 | Validation R2 0.426506
        Best loss 15.322500 | Best epoch 0014

100%|########################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([ 5.4798, 30.7803, 14.7806,  2.5093, -1.7086,  8.5024,  1.9989, -1.6791],
       grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866])

        Epoch 0015 | Training loss 12.924088 | Training R2 0.547802 | Validation loss 14.716954 | Validation R2 0.470939
        Best loss 14.716954 | Best epoch 0015

100%|########################################| 672/672 [01:31<00:00,  7.31it/s]
tensor([15.6168, 55.2221, 16.2939,  8.2661, 24.2689], grad_fn=<IndexBackward0>)
tensor([16.1690, 59.8340,  5.3050,  1.4892, 16.1690])

        Epoch 0016 | Training loss 11.898344 | Training R2 0.616732 | Validation loss 14.322660 | Validation R2 0.498908
        Best loss 14.322660 | Best epoch 0016

100%|########################################| 672/672 [01:32<00:00,  7.24it/s]
tensor([12.7216, 59.7177, 25.1669,  4.2772, 34.5799, 21.0603,  9.3780,  3.6991,
        31.5247, 18.5450,  8.8795,  3.1359, 25.5747, 15.5161,  5.9220],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018,
        65.7810, 20.9510,  4.9462,  1.6753, 64.1100, 17.0690,  4.0299])

        Epoch 0017 | Training loss 11.401729 | Training R2 0.648058 | Validation loss 13.213898 | Validation R2 0.573487
        Best loss 13.213898 | Best epoch 0017
```

```
100%|##########################################| 672/672 [01:33<00:00,  7.18it/s]
tensor([ 2.9063, 32.5171, 27.8092, 23.1816, 13.6546,  9.5199,  5.4563,  2.9917,
         0.8526, 27.3170, 15.6950,  7.0380,  3.1720, 24.6298, 14.8523,  8.5628,
         4.3510, 22.1035, 15.0576,  8.9973,  5.4540, 22.2026, 13.7354,  9.1169,
         6.3164, 22.1408, 14.2489,  9.6895,  7.1869, 21.7399, 14.4235, 10.2883,
         8.0124, 21.3545, 11.1481,  8.8666, 20.7642, 15.1376, 11.6578,  9.4312,
        20.2414, 15.3670, 12.0332, 10.2129, 21.1668, 16.4321, 13.0078, 10.8106,
        21.6568, 17.0286, 13.6380, 11.4462, 22.2054, 17.6234, 14.2651, 12.1728,
        18.4076, 15.8337], grad_fn=<IndexBackward0>)
tensor([ 2.7419, 28.6490, 21.3580, 16.8180,  8.0564,  4.9078,  2.5526,  1.5643,
         0.9587, 44.6470,  8.7898,  2.7858,  1.0463, 43.9280,  8.6592,  2.7445,
         1.0308, 44.7080,  8.8094,  2.7920,  1.0487, 45.3180,  7.5611,  2.8303,
         1.0630, 45.7270,  9.0111,  2.8560,  1.0727, 45.7350,  9.0137,  2.8568,
         1.0730, 46.3300,  2.8935,  1.0868, 44.3590,  8.7473,  2.7724,  1.0413,
        31.3930,  7.5594,  2.4035,  1.0628, 43.9420,  8.6636,  2.7459,  1.0313,
        43.7170,  8.6165,  2.7309,  1.0257, 43.3150,  8.5378,  2.7060,  1.0163,
         8.6510,  2.7419])

        Epoch 0018 | Training loss 10.813417 | Training R2 0.683441 | Validation loss 13.203379 | Validation R2 0.574166
        Best loss 13.203379 | Best epoch 0018

100%|##########################################| 672/672 [01:34<00:00,  7.12it/s]
tensor([ 9.7498, 40.5504, 13.2881,  0.8898, 25.9407, 14.4120,  2.2655,  1.0768,
        24.7947, 14.0786,  1.6502], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568])

        Epoch 0019 | Training loss 10.473630 | Training R2 0.703023 | Validation loss 13.268398 | Validation R2 0.569962
        Best loss 13.203379 | Best epoch 0018

100%|##########################################| 672/672 [01:36<00:00,  6.97it/s]
tensor([ 2.5559, 19.4985,  2.8311, 33.7559, 17.7553,  2.5439],
       grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742])

        Epoch 0020 | Training loss 9.496670 | Training R2 0.755842 | Validation loss 10.343183 | Validation R2 0.738677
        Best loss 10.343183 | Best epoch 0020

100%|##########################################| 672/672 [01:40<00:00,  6.70it/s]
tensor([ 6.5408, 27.2245, 21.7968, 17.0160, 14.4693,  9.4895, 26.6533, 19.8093,
        14.0566, 29.3762, 22.2869, 16.0390, 30.4389, 16.7182, 30.6311, 16.9595,
        30.6151, 17.0785, 30.7607, 17.0520, 30.7647, 16.8004, 30.8296, 16.6525,
        30.7940, 16.4834, 27.5907, 16.3012, 30.4290, 16.1035, 30.0555, 15.9718,
        29.7875, 15.9149, 29.5319, 15.9032, 15.8856, 26.1478, 15.8869, 28.9241,
        15.8869, 28.7300, 15.8838, 28.5423, 15.8782, 28.2471, 15.7892, 28.3878,
        15.8788, 28.1359, 23.1418], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0021 | Training loss 7.951676 | Training R2 0.828823 | Validation loss 8.662682 | Validation R2 0.816695
        Best loss 8.662682 | Best epoch 0021

100%|##########################################| 672/672 [01:47<00:00,  6.23it/s]
tensor([ 5.0714, 41.2239, 10.6933,  1.8153, -1.6648, 32.1178, 11.6598,  2.8483],
       grad_fn=<IndexBackward0>)
tensor([ 2.2708, 40.9040,  9.4533,  2.2722,  0.6695, 40.8030,  9.4476,  2.2708])

        Epoch 0022 | Training loss 7.609004 | Training R2 0.843258 | Validation loss 8.749406 | Validation R2 0.813006
        Best loss 8.662682 | Best epoch 0021

100%|##########################################| 672/672 [02:07<00:00,  5.28it/s]
tensor([ 7.4991, 41.7259, 10.5250,  2.0759, -0.8212, -0.1132],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724])

        Epoch 0023 | Training loss 6.876002 | Training R2 0.872003 | Validation loss 6.808918 | Validation R2 0.886753
        Best loss 6.808918 | Best epoch 0023

100%|##########################################| 672/672 [02:26<00:00,  4.58it/s]
tensor([10.0532, 11.7258,  3.9000, 25.9815, 11.5955,  4.2005, 24.3615, 10.3238,
         4.2509], grad_fn=<IndexBackward0>)
tensor([16.2540, 16.8150,  3.7307, 46.7120, 18.2510,  4.0494, 39.1610, 16.6890,
         4.1575])

        Epoch 0024 | Training loss 6.344456 | Training R2 0.891027 | Validation loss 6.287634 | Validation R2 0.903429
        Best loss 6.287634 | Best epoch 0024

100%|##########################################| 672/672 [02:31<00:00,  4.45it/s]
tensor([ 1.6894, 23.4610,  3.5930, -1.5898, -2.5777, 30.9283,  8.1172,  1.3945,
        -1.0457], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900])

        Epoch 0025 | Training loss 7.193916 | Training R2 0.859893 | Validation loss 8.765650 | Validation R2 0.812311
        Best loss 6.287634 | Best epoch 0024

100%|##########################################| 672/672 [02:33<00:00,  4.38it/s]
tensor([ 8.8472, 41.0249,  8.3407,  2.1899, 36.6626, 12.1595],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0026 | Training loss 6.314091 | Training R2 0.892068 | Validation loss 7.142266 | Validation R2 0.875393
        Best loss 6.287634 | Best epoch 0024

100%|##########################################| 672/672 [02:37<00:00,  4.26it/s]
tensor([ 8.5633, 52.2498,  1.5635, 17.5187,  1.9039, 16.5124,  1.4483],
       grad_fn=<IndexBackward0>)
tensor([ 5.0480, 57.3470,  1.4345, 18.1510,  1.4741, 17.6580,  1.4340])

        Epoch 0027 | Training loss 6.055744 | Training R2 0.900719 | Validation loss 5.718658 | Validation R2 0.920116
        Best loss 5.718658 | Best epoch 0027

100%|##########################################| 672/672 [02:39<00:00,  4.21it/s]
tensor([ 7.0780, 42.2500, 11.1324,  3.1023,  1.2874,  2.6817, 21.2856,  6.6037,
         3.4198], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0028 | Training loss 6.592818 | Training R2 0.882328 | Validation loss 7.770147 | Validation R2 0.852522
        Best loss 5.718658 | Best epoch 0027

100%|##########################################| 672/672 [02:38<00:00,  4.23it/s]
tensor([ 3.7971, 35.3375,  8.4819,  1.6825, -0.3244, -0.4051, 13.2231,  2.0788,
         0.1861,  0.0965, 12.3040,  2.4895,  0.1087,  0.0419],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0029 | Training loss 5.998502 | Training R2 0.902587 | Validation loss 5.604497 | Validation R2 0.923274
        Best loss 5.604497 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 1 --model 5 --save fold_1 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([2.1999, 5.6524, 5.8418, 6.1936, 9.4868, 9.8432],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521])

        Epoch 0001 | Training loss 24.587435 | Training R2 -0.636649 | Validation loss 29.936550 | Validation R2 -1.189140
        Best loss 29.936550 | Best epoch 0001

100%|##########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 4.9043,  8.9507,  9.0836,  9.2166,  9.3305, 13.3845, 13.5179, 13.6512,
        13.7654, 17.8186, 17.9522, 18.0858], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243, 63.0070, 16.7890,  4.7756])

        Epoch 0002 | Training loss 25.483650 | Training R2 -0.758136 | Validation loss 33.067993 | Validation R2 -1.671072
        Best loss 29.936550 | Best epoch 0001

100%|##########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([ 7.6014, 11.0011, 11.0285], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0003 | Training loss 24.522160 | Training R2 -0.627971 | Validation loss 32.016544 | Validation R2 -1.503911
        Best loss 29.936550 | Best epoch 0001

100%|##########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 7.3291, 10.1608, 10.0233,  9.8829], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.401255 | Training R2 -0.358544 | Validation loss 28.629280 | Validation R2 -1.002123
        Best loss 28.629280 | Best epoch 0004

100%|##########################################| 672/672 [01:29<00:00,  7.53it/s]
```

```
tensor([14.4474, 19.8099, 19.4276, 18.6136, 23.0821, 21.7736, 26.9981, 26.1418,
        24.3684, 28.5206, 26.5152], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836])

        Epoch 0005 | Training loss 19.169922 | Training R2 0.005122 | Validation loss 21.290998 | Validation R2 -0.107291
        Best loss 21.290998 | Best epoch 0005

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([12.2309, 18.9201, 18.0805, 16.3241, 20.7797, 18.8313, 22.8460, 20.6343,
        24.4485, 21.9717], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0006 | Training loss 19.678331 | Training R2 -0.048349 | Validation loss 22.492300 | Validation R2 -0.235770
        Best loss 21.290998 | Best epoch 0005

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([ 9.0321, 16.7148, 15.5704, 14.4203], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0007 | Training loss 18.438383 | Training R2 0.079604 | Validation loss 20.871935 | Validation R2 -0.064132
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 0.2794,  0.7751,  0.5484, -0.3596, -1.8415, -1.9520, -2.6358, -3.3204,
        -2.3768, -4.0057, -5.6395], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0008 | Training loss 20.370321 | Training R2 -0.123375 | Validation loss 23.957869 | Validation R2 -0.402059
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([17.7417, 27.3907, 25.9303], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0009 | Training loss 19.084763 | Training R2 0.013942 | Validation loss 21.900980 | Validation R2 -0.171647
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([17.3056, 25.6101, 24.2517, 20.7280, 26.5591, 24.9605, 21.8946, 26.8496,
        25.2540, 22.2393], grad_fn=<IndexBackward0>)
tensor([17.8830, 55.3190, 16.9870,  2.1271, 56.8470, 17.5230,  2.1942, 57.7130,
        17.7900,  2.2277])

        Epoch 0010 | Training loss 17.859404 | Training R2 0.136499 | Validation loss 20.114540 | Validation R2 0.011697
        Best loss 20.114540 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 8.7530, 19.8132, 16.8510, 16.2882, 22.7456, 19.5403, 19.2723],
       grad_fn=<IndexBackward0>)
tensor([ 9.2660, 25.5950,  5.0055,  3.7205, 26.2690,  4.4291,  3.8185])

        Epoch 0011 | Training loss 18.237335 | Training R2 0.099566 | Validation loss 20.373814 | Validation R2 -0.013945
        Best loss 20.114540 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 9.9975, 15.6876, 13.4450, 11.2903, 17.1275, 15.1765, 11.2384],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727])

        Epoch 0012 | Training loss 17.548340 | Training R2 0.166316 | Validation loss 19.443098 | Validation R2 0.076577
        Best loss 19.443098 | Best epoch 0012

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 9.9177, 18.4395, 17.9721, 17.5216, 14.3823, 12.5939, 11.2551,  9.9186,
        16.4753, 13.8464], grad_fn=<IndexBackward0>)
tensor([ 4.1835, 35.5470, 29.2780, 24.3620,  6.9018,  3.3599,  1.9581,  1.1412,
        14.7460,  4.1835])

        Epoch 0013 | Training loss 17.206947 | Training R2 0.198439 | Validation loss 19.141432 | Validation R2 0.105009
        Best loss 19.141432 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([12.4364, 27.2565, 23.2694, 19.6116, 16.4919, 29.9886, 27.1892, 23.8359,
        20.2024], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243])

        Epoch 0014 | Training loss 17.306837 | Training R2 0.189105 | Validation loss 19.362793 | Validation R2 0.084189
        Best loss 19.141432 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([ 9.0598, 20.0499, 19.4907, 18.9320, 17.8166, 16.1479, 12.2752, 10.0752,
         8.9788, 18.8787, 14.2877, 10.3545,  8.6562, 18.4221, 14.3182, 10.7028,
         9.1701], grad_fn=<IndexBackward0>)
tensor([ 1.7205, 44.0430, 33.8580, 27.3170, 18.5670, 10.6030,  2.8810,  1.3684,
         0.9431, 27.6900,  6.1533,  1.6721,  0.9567, 23.0690,  6.2359,  1.6946,
         0.9695])

        Epoch 0015 | Training loss 16.755896 | Training R2 0.239911 | Validation loss 19.031542 | Validation R2 0.115256
        Best loss 19.031542 | Best epoch 0015

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([  0.9582,   1.0904,   0.4565,  -1.8299,  -3.4424,  -5.5529,  -7.1404,
        -8.7248,  -7.3052, -10.9318, -14.4289], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0016 | Training loss 16.645119 | Training R2 0.249928 | Validation loss 18.393700 | Validation R2 0.173566
        Best loss 18.393700 | Best epoch 0016

100%|########################################| 672/672 [01:33<00:00,  7.20it/s]
tensor([ 6.8242, 20.9803, 15.5757, 10.6441,  6.5071, 20.2602, 15.3891, 10.3295,
         6.6992, 19.2614, 16.2280, 12.1368,  8.1876], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581])

        Epoch 0017 | Training loss 16.093096 | Training R2 0.298854 | Validation loss 17.970434 | Validation R2 0.211163
        Best loss 17.970434 | Best epoch 0017

100%|########################################| 672/672 [01:37<00:00,  6.88it/s]
tensor([12.8932, 35.1585, 29.2565, 17.6236, 35.2379, 31.1231, 21.2395],
       grad_fn=<IndexBackward0>)
tensor([ 3.8765, 62.3080, 16.2100,  1.3937, 63.5960, 16.5530,  1.4231])

        Epoch 0018 | Training loss 15.311383 | Training R2 0.365315 | Validation loss 16.984724 | Validation R2 0.295328
        Best loss 16.984724 | Best epoch 0018

100%|########################################| 672/672 [01:48<00:00,  6.19it/s]
tensor([16.5482, 29.7475, 28.0376], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0019 | Training loss 14.230635 | Training R2 0.451751 | Validation loss 15.854136 | Validation R2 0.386019
        Best loss 15.854136 | Best epoch 0019

100%|########################################| 672/672 [02:01<00:00,  5.51it/s]
tensor([19.7466, 42.1145, 30.2606, 14.1118, 37.6893, 25.5962, 11.4744, 34.7414,
        11.2551, 33.2510, 23.2312, 11.2077, 33.0895, 23.2144, 11.2046, 32.8959,
        23.1463, 11.2140, 32.9500, 23.3397, 11.3844, 32.9221, 23.4265, 11.5103,
        23.5826, 11.6663, 32.9310, 23.6521, 11.7840, 32.9144, 23.7639],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0020 | Training loss 12.025496 | Training R2 0.608497 | Validation loss 13.721763 | Validation R2 0.540072
        Best loss 13.721763 | Best epoch 0020

100%|########################################| 672/672 [02:24<00:00,  4.66it/s]
tensor([11.1434, 49.1650, 25.8507, 12.7483], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0021 | Training loss 12.230107 | Training R2 0.595061 | Validation loss 13.446256 | Validation R2 0.558356
        Best loss 13.446256 | Best epoch 0021

100%|########################################| 672/672 [02:39<00:00,  4.20it/s]
tensor([ 7.8498, 35.5636, 31.8140, 27.4297, 23.8189, 15.3497, 39.8910, 28.7233,
        18.5893, 41.4949, 30.8928, 19.8995, 41.8754, 38.6326, 20.1299, 38.6822,
        20.5340, 38.5935, 21.5521], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590])

        Epoch 0022 | Training loss 9.790716 | Training R2 0.740488 | Validation loss 12.751149 | Validation R2 0.602837
        Best loss 12.751149 | Best epoch 0022

100%|########################################| 672/672 [02:37<00:00,  4.28it/s]
tensor([14.1666, 61.5551, 29.6613,  8.8076, 58.5753, 24.2845,  8.8832],
       grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781])

        Epoch 0023 | Training loss 8.497423 | Training R2 0.804519 | Validation loss 10.855521 | Validation R2 0.712147
        Best loss 10.855521 | Best epoch 0023

100%|########################################| 672/672 [02:45<00:00,  4.06it/s]
tensor([15.8495, 61.9667, 28.1483, 10.4488], grad_fn=<IndexBackward0>)
tensor([18.4370, 63.6710, 21.1850,  2.2930])

        Epoch 0024 | Training loss 7.026572 | Training R2 0.866335 | Validation loss 7.219308 | Validation R2 0.872690
        Best loss 7.219308 | Best epoch 0024

100%|########################################| 672/672 [03:02<00:00,  3.68it/s]
tensor([15.0177, 53.2453, 22.2480, 13.1297, 52.0899, 24.2600],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])
```

```
        Epoch 0025 | Training loss 22.096283 | Training R2 -0.321805 | Validation loss 31.622337 | Validation R2 -1.442631
        Best loss 7.219308 | Best epoch 0024

100%|########################################| 672/672 [02:59<00:00,  3.75it/s]
tensor([ 9.0573, 64.8458, 19.9370,  7.2607,  4.3328, 59.8810, 18.9035,  3.8537],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0026 | Training loss 6.403774 | Training R2 0.888980 | Validation loss 6.044273 | Validation R2 0.910760
        Best loss 6.044273 | Best epoch 0026

100%|########################################| 672/672 [02:57<00:00,  3.79it/s]
tensor([ 6.9223, 61.5160, 18.7082,  3.0362, 18.1905,  2.9401, 18.2441,  2.8033],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559])

        Epoch 0027 | Training loss 6.205529 | Training R2 0.895747 | Validation loss 6.115032 | Validation R2 0.908659
        Best loss 6.044273 | Best epoch 0026

100%|########################################| 672/672 [02:57<00:00,  3.80it/s]
tensor([ 6.6950, 60.9784, 50.3774, 41.8519, 28.7659, 16.2084,  8.8678,  3.7320,
         2.6390], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0028 | Training loss 6.358976 | Training R2 0.890528 | Validation loss 5.888662 | Validation R2 0.915296
        Best loss 5.888662 | Best epoch 0028

100%|########################################| 672/672 [02:54<00:00,  3.85it/s]
tensor([ 5.4355, 52.7556, 12.8180,  2.5391], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0029 | Training loss 6.320073 | Training R2 0.891863 | Validation loss 5.790334 | Validation R2 0.918101
        Best loss 5.790334 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 2 --model 1 --save fold_2 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([2.2012, 4.3401, 4.5154, 4.6905, 4.8404, 7.3129, 9.4333, 9.6325, 9.8317],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0001 | Training loss 24.396061 | Training R2 -0.611271 | Validation loss 29.565437 | Validation R2 -1.135200
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 4.5868,  7.7243,  7.7393,  7.7542,  7.7692,  7.8141, 10.7971, 10.8420,
        10.8870, 13.8658, 13.9107, 13.9557, 16.8932, 16.9082, 16.9831, 19.9356,
        20.0105, 22.9630, 23.0379, 26.0379, 29.0378, 31.9629, 32.0378,
        34.8668, 34.9417, 37.7557, 37.8606], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590, 15.2690, 43.9280, 15.2390, 35.5910, 15.2300,
        34.7690, 14.8850, 42.5860, 12.5700])

        Epoch 0002 | Training loss 25.662014 | Training R2 -0.782833 | Validation loss 33.517918 | Validation R2 -1.744252
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.62it/s]
tensor([5.6275, 8.8024, 8.7686], grad_fn=<IndexBackward0>)
tensor([ 2.9348, 49.9070,  2.9348])

        Epoch 0003 | Training loss 24.307240 | Training R2 -0.599560 | Validation loss 31.725683 | Validation R2 -1.458623
        Best loss 29.565437 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 7.0766, 10.0451,  9.7717,  9.5309,  9.2409, 11.8985, 11.5903, 11.2770,
        11.0037], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197])

        Epoch 0004 | Training loss 19.475636 | Training R2 -0.026863 | Validation loss 22.108311 | Validation R2 -0.193936
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([15.8276, 23.3258, 22.6143], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0005 | Training loss 20.458645 | Training R2 -0.133138 | Validation loss 24.160664 | Validation R2 -0.425895
        Best loss 22.108311 | Best epoch 0004

100%|########################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 9.2572, 13.8954, 12.9740], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0006 | Training loss 17.644037 | Training R2 0.157199 | Validation loss 18.924053 | Validation R2 0.125221
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 6.5554, 14.4303, 14.2323, 14.0333, 13.2285, 12.6145, 11.7806, 11.1425],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0007 | Training loss 17.723608 | Training R2 0.149580 | Validation loss 19.722084 | Validation R2 0.049886
        Best loss 18.924053 | Best epoch 0006

100%|########################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([17.9146, 28.9038, 27.0520, 23.5514, 30.4003, 28.1080, 23.7917, 29.1836,
        26.5059, 21.4689, 25.4389, 22.4455, 17.6895, 16.8178, 19.2722],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.6890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775, 17.6690])

        Epoch 0008 | Training loss 16.884079 | Training R2 0.228237 | Validation loss 18.234676 | Validation R2 0.187794
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([17.3961, 35.1640, 32.7303], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0009 | Training loss 17.305775 | Training R2 0.189205 | Validation loss 20.149847 | Validation R2 0.008224
        Best loss 18.234676 | Best epoch 0008

100%|########################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([ 0.9194,  2.6580,  2.2602,  1.8612,  1.4610, -0.2532, -1.1996, -1.9260,
        -2.2793], grad_fn=<IndexBackward0>)
tensor([0.3554, 5.3208, 4.0322, 3.2185, 2.6321, 1.2520, 0.7242, 0.3492, 0.2020])

        Epoch 0010 | Training loss 16.073269 | Training R2 0.300581 | Validation loss 18.079575 | Validation R2 0.201553
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([21.2469, 44.4680, 39.3766, 29.7086, 36.6719, 24.5128],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441])

        Epoch 0011 | Training loss 16.631989 | Training R2 0.251111 | Validation loss 19.968565 | Validation R2 0.025990
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([-0.2112,  9.6766,  8.9151,  3.7237,  1.2923], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0012 | Training loss 16.117798 | Training R2 0.296700 | Validation loss 19.308783 | Validation R2 0.089291
        Best loss 18.079575 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 8.1193, 28.2361, 13.4984], grad_fn=<IndexBackward0>)
tensor([ 2.9348, 49.9070,  2.9348])

        Epoch 0013 | Training loss 15.069706 | Training R2 0.385193 | Validation loss 17.587860 | Validation R2 0.244393
        Best loss 17.587860 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([28.5283, 47.7753, 46.5215, 45.2703, 44.0218, 39.0541, 35.3557, 30.4602,
        26.8148, 23.1959, 40.9320, 28.8364, 19.7065, 14.5983],
       grad_fn=<IndexBackward0>)
tensor([50.4930, 47.4530, 35.8760, 28.7780, 23.7390, 11.8000,  7.0637,  3.5658,
         2.1356,  1.2790, 48.6290, 12.1880,  3.6833,  1.3211])

        Epoch 0014 | Training loss 13.840353 | Training R2 0.481411 | Validation loss 15.888102 | Validation R2 0.383385
        Best loss 15.888102 | Best epoch 0014

100%|########################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([19.5747, 57.5473, 43.1012, 17.4868, 42.4553, 25.7603, 14.2486, 30.5511,
        15.0762, 24.2108, 19.7464], grad_fn=<IndexBackward0>)
tensor([17.5830, 71.0850, 22.2940,  2.9600, 49.2230, 14.1200,  2.9876, 52.3580,
         3.1778, 44.7320, 17.5830])

        Epoch 0015 | Training loss 13.451623 | Training R2 0.510133 | Validation loss 15.478939 | Validation R2 0.414735
```

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        Best loss 15.478939 | Best epoch 0015

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([15.3390, 40.8979, 27.4991,  6.8975, 27.3409, 16.6550],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0016 | Training loss 12.981250 | Training R2 0.543793 | Validation loss 14.996788 | Validation R2 0.450628
        Best loss 14.996788 | Best epoch 0016

100%|########################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([20.6242, 87.1770, 56.6517], grad_fn=<IndexBackward0>)
tensor([12.6410, 93.0030, 31.3750])

        Epoch 0017 | Training loss 12.344368 | Training R2 0.587459 | Validation loss 14.402932 | Validation R2 0.493276
        Best loss 14.402932 | Best epoch 0017

100%|########################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([ 5.8743, 33.4952, 14.7101,  2.2171, -1.6118, -3.1793, 19.0814,  7.9290,
         2.0781, -3.3863,  6.3008,  0.5193, -5.0548], grad_fn=<IndexBackward0>)
tensor([ 3.4332, 50.3360, 16.1560,  3.8901,  1.9088,  1.3372, 50.8530, 13.6880,
         5.6217,  1.3536, 19.2430,  5.5348,  1.1154])

        Epoch 0018 | Training loss 11.731128 | Training R2 0.627429 | Validation loss 13.635745 | Validation R2 0.545820
        Best loss 13.635745 | Best epoch 0018

100%|########################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([ 9.1925, 60.4866, 25.4927,  2.9691, 22.6411,  3.5867, 18.8998,  2.9576,
        16.7243,  2.9704], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0019 | Training loss 11.256901 | Training R2 0.656943 | Validation loss 13.020782 | Validation R2 0.585863
        Best loss 13.020782 | Best epoch 0019

100%|########################################| 672/672 [01:33<00:00,  7.19it/s]
tensor([13.8924, 49.3759, 17.0867,  2.1433, 32.8296, 15.3211,  1.6264],
       grad_fn=<IndexBackward0>)
tensor([14.0340, 52.5400, 13.3690,  1.8996, 54.8650, 14.0150,  1.9913])

        Epoch 0020 | Training loss 10.266763 | Training R2 0.714638 | Validation loss 12.052997 | Validation R2 0.645138
        Best loss 12.052997 | Best epoch 0020

100%|########################################| 672/672 [01:34<00:00,  7.09it/s]
tensor([ 1.2734, 12.3216, -0.0398,  9.7799,  0.8759], grad_fn=<IndexBackward0>)
tensor([0.1803, 6.8826, 0.1879, 5.1060, 0.1803])

        Epoch 0021 | Training loss 9.368041 | Training R2 0.762411 | Validation loss 10.987734 | Validation R2 0.705092
        Best loss 10.987734 | Best epoch 0021

100%|########################################| 672/672 [01:37<00:00,  6.87it/s]
tensor([ 2.8928,  7.5500,  1.0634, -2.5524, 21.9355,  8.8222,  1.5529, -0.8570,
        -1.7677,  8.2143,  4.1006, -1.0089], grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625, 15.0820,  8.0548,  1.9640])

        Epoch 0022 | Training loss 8.574180 | Training R2 0.800972 | Validation loss 9.521894 | Validation R2 0.778529
        Best loss 9.521894 | Best epoch 0022

100%|########################################| 672/672 [01:42<00:00,  6.53it/s]
tensor([11.8306, 63.7298, 21.1029,  1.9694, 50.4705, 22.5680,  4.1765, 49.5880,
        23.2013, 11.2773,  6.1622], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])

        Epoch 0023 | Training loss 8.035305 | Training R2 0.825203 | Validation loss 9.607019 | Validation R2 0.774552
        Best loss 9.521894 | Best epoch 0022

100%|########################################| 672/672 [01:58<00:00,  5.66it/s]
tensor([ 6.3880, 14.1343,  2.3735, 29.4463, 13.7770,  2.6396, 30.1243, 13.3924,
         2.9050, 30.8156, 13.5442,  3.0128, 30.5357, 13.4501],
       grad_fn=<IndexBackward0>)
tensor([ 9.8032,  9.6259,  0.6383, 43.8570,  9.7042,  0.6435, 44.0790,  9.7534,
         0.6467, 44.4320,  9.8362,  0.6522, 44.3040,  9.8032])

        Epoch 0024 | Training loss 7.263038 | Training R2 0.857188 | Validation loss 8.324299 | Validation R2 0.830736
        Best loss 8.324299 | Best epoch 0024

100%|########################################| 672/672 [02:15<00:00,  4.95it/s]
tensor([26.6158, 57.6124], grad_fn=<IndexBackward0>)
tensor([47.8150, 46.0380])

        Epoch 0025 | Training loss 6.618134 | Training R2 0.881423 | Validation loss 6.747346 | Validation R2 0.888792
        Best loss 6.747346 | Best epoch 0025

100%|########################################| 672/672 [02:24<00:00,  4.65it/s]
tensor([ 8.1440, 64.3160, 18.0991,  0.7626, 17.8471,  1.6511, 16.7843,  1.7408,
        16.2581,  1.1391], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0026 | Training loss 6.682505 | Training R2 0.879105 | Validation loss 6.442039 | Validation R2 0.898628
        Best loss 6.442039 | Best epoch 0026

100%|########################################| 672/672 [02:28<00:00,  4.52it/s]
tensor([ 3.0113, 11.6365,  1.9527], grad_fn=<IndexBackward0>)
tensor([2.0948, 9.5297, 2.0948])

        Epoch 0027 | Training loss 6.799114 | Training R2 0.874849 | Validation loss 6.605771 | Validation R2 0.893410
        Best loss 6.442039 | Best epoch 0026

100%|########################################| 672/672 [02:31<00:00,  4.43it/s]
tensor([10.0965, 64.9965, 18.0683,  2.7577, 49.3049, 19.3117,  7.8974,  5.1164],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018])

        Epoch 0028 | Training loss 7.477236 | Training R2 0.848640 | Validation loss 9.610397 | Validation R2 0.774393
        Best loss 6.442039 | Best epoch 0026

100%|########################################| 672/672 [02:33<00:00,  4.38it/s]
tensor([ 6.7122, 47.8820, 13.4944,  2.2469], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0029 | Training loss 6.323672 | Training R2 0.891740 | Validation loss 5.862009 | Validation R2 0.916061
        Best loss 5.862009 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 2 --model 2 --save fold_2 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:27<00:00,  7.69it/s]
tensor([ 2.1615,  4.8593,  5.0546,  5.4167,  7.8210,  8.3762, 10.8642, 11.1145,
        11.2536, 13.7084, 14.0987], grad_fn=<IndexBackward0>)
tensor([ 7.7458, 46.1910, 15.8890,  2.9155, 46.8330,  2.9904, 18.0300,  5.5715,
         2.9028, 17.7490,  2.8574])

        Epoch 0001 | Training loss 25.062193 | Training R2 -0.700463 | Validation loss 31.127050 | Validation R2 -1.366714
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:27<00:00,  7.70it/s]
tensor([4.8389, 7.9815, 8.0795, 8.1939], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0002 | Training loss 25.686121 | Training R2 -0.786184 | Validation loss 33.511566 | Validation R2 -1.743212
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([10.7876, 14.7278, 14.7281, 14.7284, 14.7289, 14.7298, 14.7307, 14.7318,
        14.7326], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0003 | Training loss 24.546101 | Training R2 -0.631151 | Validation loss 32.111191 | Validation R2 -1.518737
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:27<00:00,  7.71it/s]
tensor([3.3280, 8.1569], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0004 | Training loss 22.813705 | Training R2 -0.409032 | Validation loss 29.552938 | Validation R2 -1.133395
        Best loss 29.552938 | Best epoch 0004

100%|########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([2.0743, 3.6892, 3.5648, 3.4382, 3.1781, 2.7698, 2.3375, 1.7664, 1.4013],
       grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0005 | Training loss 18.439297 | Training R2 0.079513 | Validation loss 20.436989 | Validation R2 -0.020243
        Best loss 20.436989 | Best epoch 0005

100%|########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([14.8184, 21.9938, 21.1540, 19.1529, 25.6132, 24.3171, 21.8638, 28.2239,
        26.6049, 23.5441, 29.8066, 27.8578, 24.1761], grad_fn=<IndexBackward0>)
```

```
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781, 68.7910,
        23.4760,  4.5602, 68.2770, 23.3020,  4.5263])

        Epoch 0006 | Training loss 17.760878 | Training R2 0.146000 | Validation loss 19.276941 | Validation R2 0.092292
        Best loss 19.276941 | Best epoch 0006

100%|##########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 7.2685, 17.8126, 17.6222, 17.4313, 16.6626, 16.0806, 15.2971, 14.1049,
         19.7325, 18.0599, 16.3651], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0007 | Training loss 17.224669 | Training R2 0.196787 | Validation loss 18.606171 | Validation R2 0.154363
        Best loss 18.606171 | Best epoch 0007

100%|##########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 8.3480, 18.9609, 17.0796, 13.5076, 19.1425, 16.7568, 12.2467, 17.5037,
        15.0191,  9.3061, 14.1835, 11.0108], grad_fn=<IndexBackward0>)
tensor([ 4.9161, 42.0730,  5.4589, 60.7050, 39.7010,  5.1625,  0.1270, 38.5530,
         6.6617,  0.1233, 37.8370,  4.9161])

        Epoch 0008 | Training loss 16.808960 | Training R2 0.235089 | Validation loss 18.387007 | Validation R2 0.174167
        Best loss 18.387007 | Best epoch 0008

100%|##########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([ 5.5405, 18.0450, 15.2522, 13.2369, 12.8317, 18.4610, 14.6685, 11.4213,
        11.8837, 10.3732, 10.1442, 13.0661, 11.2028,  9.8967,  9.6595],
       grad_fn=<IndexBackward0>)
tensor([ 9.8083, 13.5140,  3.7950,  1.5319,  1.2778, 13.2800,  3.7295,  1.2557,
         3.7290,  1.5053,  1.2555, 13.1880,  3.7035,  1.4950,  1.2470])

        Epoch 0009 | Training loss 16.176075 | Training R2 0.291605 | Validation loss 17.658480 | Validation R2 0.238313
        Best loss 17.658480 | Best epoch 0009

100%|##########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([ 4.4795, 11.8215,  9.0239,  6.1657, 12.2526,  8.1955,  6.0050,  5.2888,
         5.0226], grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625])

        Epoch 0010 | Training loss 15.784349 | Training R2 0.325499 | Validation loss 17.559269 | Validation R2 0.246848
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([12.7334, 35.1197, 29.4521, 23.7096, 18.7326, 32.3226, 24.1075],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0011 | Training loss 19.306719 | Training R2 -0.009128 | Validation loss 25.415319 | Validation R2 -0.577833
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([32.0389, 42.7443, 41.9388, 41.1327, 39.5190, 37.9050, 47.3776, 44.0538,
        40.7275, 49.5277, 43.8861, 41.0659, 49.2414, 39.0088, 46.8657, 34.8696,
        42.4265, 29.7071, 36.3832, 27.1146, 31.6529, 26.3287, 30.2598, 25.4065],
       grad_fn=<IndexBackward0>)
tensor([58.5520, 41.9580, 32.6790, 27.1470, 20.1960, 15.4500, 55.2420, 32.3270,
        21.5820, 60.6230, 31.3470, 24.0360, 61.8120, 24.6620, 62.3610, 24.9130,
        62.5810, 25.0130, 62.4280, 24.9640, 62.3850, 24.9450, 62.3680, 24.9370])

        Epoch 0012 | Training loss 15.314219 | Training R2 0.365080 | Validation loss 18.021051 | Validation R2 0.206713
        Best loss 17.559269 | Best epoch 0010

100%|##########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([ 0.5030,  2.0243,  1.2888,  0.5755,  0.0550, -1.1188, -1.4900, -1.7581,
        -1.9126, -2.0494, -1.1390, -1.4614, -1.5448, -1.7284, -1.9236],
       grad_fn=<IndexBackward0>)
tensor([0.1027, 4.3675, 3.3207, 2.6789, 2.2198, 1.1160, 0.6726, 0.3426, 0.2066,
        0.1245, 4.4427, 1.1442, 0.8164, 0.3513, 0.1277])

        Epoch 0013 | Training loss 14.627570 | Training R2 0.420740 | Validation loss 16.876558 | Validation R2 0.304275
        Best loss 16.876558 | Best epoch 0013

100%|##########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([ 8.8011, 44.5529, 42.7156, 40.8827, 31.7829, 26.4018, 19.3116,  9.0496,
        38.4039, 23.2554, 15.9224, 11.0489, 20.7719, 15.0965, 11.2353, 18.4193,
        15.1102, 12.8798, 18.1327, 16.6533, 15.1084, 19.4565, 18.0770, 16.5790,
        18.9628], grad_fn=<IndexBackward0>)
tensor([ 4.2877, 59.4320, 46.9050, 38.1280, 14.2580,  7.9220,  3.6186,  1.1171,
        59.4890, 17.3990,  4.4157,  1.1207, 17.1950,  4.3640,  1.1075, 17.2810,
         4.3856,  1.1130, 16.8630,  5.2057,  1.0861, 16.8560,  4.2779,  1.0857,
         4.2077])

        Epoch 0014 | Training loss 13.552494 | Training R2 0.502758 | Validation loss 15.915753 | Validation R2 0.381237
        Best loss 15.915753 | Best epoch 0014

100%|##########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 4.4982, 21.3597,  5.1706], grad_fn=<IndexBackward0>)
tensor([ 4.6703, 20.6660,  3.8425])

        Epoch 0015 | Training loss 13.312044 | Training R2 0.520246 | Validation loss 15.572647 | Validation R2 0.407628
        Best loss 15.572647 | Best epoch 0015

100%|##########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 5.1438,  8.7150,  8.2335, 17.3058, 10.0088,  9.1330, 17.2026, 10.6696,
        10.4114], grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462])

        Epoch 0016 | Training loss 12.642657 | Training R2 0.567281 | Validation loss 14.518663 | Validation R2 0.485100
        Best loss 14.518663 | Best epoch 0016

100%|##########################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([ 8.6458, 39.9109, 19.5235,  1.5698, 25.5519, 13.4577,  2.6799],
       grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173])

        Epoch 0017 | Training loss 12.009523 | Training R2 0.609536 | Validation loss 13.955899 | Validation R2 0.524243
        Best loss 13.955899 | Best epoch 0017

100%|##########################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([16.5268, 53.2245, 25.6311,  4.3723, 32.4923, 17.3056,  3.8944, 25.6408,
        15.9058,  4.0992], grad_fn=<IndexBackward0>)
tensor([12.3700, 69.3770, 19.4920,  2.1362, 68.1120, 16.1970,  2.1042, 46.9250,
        16.8400,  2.1878])

        Epoch 0018 | Training loss 11.491714 | Training R2 0.642481 | Validation loss 14.003984 | Validation R2 0.520958
        Best loss 13.955899 | Best epoch 0017

100%|##########################################| 672/672 [01:31<00:00,  7.31it/s]
tensor([12.2880, 60.9434, 23.6948,  3.7652, 41.1423, 23.2139,  4.3050, 37.7644,
        21.6612, 10.9115,  4.7921, 33.1801, 17.9587,  9.4201,  4.5785],
       grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370, 62.9420, 16.8690,  6.5668,  3.3492])

        Epoch 0019 | Training loss 10.620493 | Training R2 0.694636 | Validation loss 12.171548 | Validation R2 0.638123
        Best loss 12.171548 | Best epoch 0019

100%|##########################################| 672/672 [01:32<00:00,  7.23it/s]
tensor([17.7791, 60.7902, 21.8121,  3.3622, 36.1535, 18.7518,  3.8016, 34.5173,
        18.5345,  3.7166], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0020 | Training loss 9.667159 | Training R2 0.746996 | Validation loss 11.243977 | Validation R2 0.691177
        Best loss 11.243977 | Best epoch 0020

100%|##########################################| 672/672 [01:35<00:00,  7.07it/s]
tensor([ 6.4277, 43.8652, 10.8547,  0.8505], grad_fn=<IndexBackward0>)
tensor([ 1.7780, 53.9210, 16.2500,  5.2152])

        Epoch 0021 | Training loss 9.009152 | Training R2 0.780266 | Validation loss 9.978053 | Validation R2 0.756801
        Best loss 9.978053 | Best epoch 0021

100%|##########################################| 672/672 [01:38<00:00,  6.83it/s]
tensor([ 7.1529, 44.6963, 12.5524,  2.6736, -0.6076, -1.8314, 12.8853,  3.2542,
         0.2715, -0.8585, 10.7207,  4.6728,  1.5571,  0.3938],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8004,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0022 | Training loss 8.104481 | Training R2 0.822180 | Validation loss 8.888013 | Validation R2 0.807035
        Best loss 8.888013 | Best epoch 0022

100%|##########################################| 672/672 [01:43<00:00,  6.47it/s]
tensor([ 9.0191, 62.1389,  0.5210, -0.0926,  2.1431], grad_fn=<IndexBackward0>)
tensor([ 2.7853, 66.9550,  2.7495,  2.3342,  2.7853])

        Epoch 0023 | Training loss 8.010061 | Training R2 0.826300 | Validation loss 9.681182 | Validation R2 0.771057
        Best loss 8.888013 | Best epoch 0022

100%|##########################################| 672/672 [01:56<00:00,  5.77it/s]
tensor([ 3.4122,  6.5380,  0.7621, -1.5433, 25.6093,  7.9584,  1.0656, -0.6848,
        -1.0974,  7.6864,  3.0400, -1.3328, 15.6097,  3.6924, -0.7531, -1.4187,
        17.5918,  4.1631, -0.1998, -1.6550, 11.6587, -1.1651, -2.1033, 22.8726,
         5.6386, -0.3096, -2.2767, 22.2590,  5.2173, -0.8715, -2.5756, 21.4615,
         3.5346, -1.2039, -2.7982, 20.7264,  1.8163, -2.2834],
       grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625, 15.0820,  8.0548,  1.9640, 29.0970,  9.7026,  3.2372,  2.0224,
        33.9450, 11.2970,  4.4089,  2.0129, 24.7420,  3.7684,  2.0126, 48.9190,
        15.4550,  5.1565,  2.0125, 48.9190, 15.4550,  5.1565,  2.0125, 48.9190,
        13.2120,  5.1565,  2.0125, 48.9190, 11.2950,  3.7684])

        Epoch 0024 | Training loss 7.332561 | Training R2 0.854441 | Validation loss 7.375947 | Validation R2 0.867106
        Best loss 7.375947 | Best epoch 0024

100%|##########################################| 672/672 [02:15<00:00,  4.97it/s]
```

```
tensor([17.5115, 75.5686, 24.1151,  5.0300, 47.8906, 15.6807,  4.7381, 48.6322,
         3.4479, 40.0268, 15.2362], grad_fn=<IndexBackward0>)
tensor([17.5830, 71.0850, 22.2940,  2.9600, 49.2230, 14.1200,  2.9876, 52.3580,
         3.1778, 44.7320, 17.5830])

        Epoch 0025 | Training loss 8.509421 | Training R2 0.803967 | Validation loss 9.115965 | Validation R2 0.797010
        Best loss 7.375947 | Best epoch 0024

100%|########################################| 672/672 [02:22<00:00,  4.72it/s]
tensor([ 9.7489, 43.1830, 33.0272, 24.0184, 12.7075,  8.0704,  4.5794,  2.5688,
        37.6630, 14.1537,  6.5239,  4.7297, 40.0373, 15.7862,  7.8193,  6.2941,
        41.6687, 24.4670,  7.7723,  7.5809, 42.2466, 14.8588, 10.3533,  8.6096,
        42.5899, 18.5460, 11.0454,  9.2425, 43.5388, 17.5699, 11.5147,  9.8455,
        44.1187, 19.8935, 11.9677, 10.3997, 44.5415, 20.4890],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385,
        43.0630, 20.8330,  1.9210,  1.3667, 43.0860,  8.8969,  3.7979,  1.3674,
        42.5380, 12.3470,  3.7496,  1.3500, 42.9850, 10.5230,  3.7888,  1.3642,
        43.0840, 12.5050,  3.7977,  1.3674, 43.0840, 12.5050])

        Epoch 0026 | Training loss 7.642862 | Training R2 0.841860 | Validation loss 9.652371 | Validation R2 0.772418
        Best loss 7.375947 | Best epoch 0024

100%|########################################| 672/672 [02:25<00:00,  4.62it/s]
tensor([ 8.1295, 16.1995,  3.9024, 38.7570, 16.0048], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0027 | Training loss 6.217919 | Training R2 0.895331 | Validation loss 6.709231 | Validation R2 0.890045
        Best loss 6.709231 | Best epoch 0027

100%|########################################| 672/672 [02:29<00:00,  4.50it/s]
tensor([ 2.9591, 16.0822,  0.4870, 41.0720, 13.1148,  0.7645, 43.0557, 15.5036,
         2.9654,  1.1200, 14.4833,  3.8689,  1.5330, 17.2718,  4.1735,  2.0491,
         5.0674,  2.6229,  7.1752,  3.4310, 51.3981,  6.0681,  3.6774,  8.0776,
         4.6272, 41.4533,  7.2080,  4.7518], grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742, 43.9160, 13.4380,
         2.8234,  1.0649, 12.6990,  3.2428,  1.0064, 15.4190,  3.2397,  1.0054,
         3.3101,  1.0273,  4.8677,  1.0228, 53.4230,  3.3111,  1.0275,  4.8942,
         1.0283, 40.7690,  3.8721,  0.9887])

        Epoch 0028 | Training loss 6.206502 | Training R2 0.895715 | Validation loss 7.057861 | Validation R2 0.878321
        Best loss 6.709231 | Best epoch 0027

100%|########################################| 672/672 [02:30<00:00,  4.46it/s]
tensor([ 7.6626, 77.2475, 59.0601, 48.7603, 39.5699, 12.5270,  0.4892, -2.0569,
        -3.5056, 59.4931, 14.3282,  1.8468, -1.0112, 59.4113, 14.9668,  2.1448,
        -0.3603, 60.1407, 15.7482,  2.9394,  0.3238], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947, 73.8930, 26.4440, 10.0160,
         5.0069, 74.0470, 26.5260, 10.0480,  5.0226])

        Epoch 0029 | Training loss 5.844729 | Training R2 0.907518 | Validation loss 5.710489 | Validation R2 0.920344
        Best loss 5.710489 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 2 --model 3 --save fold_2 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:27<00:00,  7.64it/s]
tensor([ 2.8156,  6.4742,  6.6527,  6.8312,  6.9842, 10.4804, 10.6588],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0001 | Training loss 25.589478 | Training R2 -0.772768 | Validation loss 32.346756 | Validation R2 -1.555826
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:27<00:00,  7.66it/s]
tensor([1.9038, 5.0573, 5.0673, 5.1375, 5.1977], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0002 | Training loss 25.551172 | Training R2 -0.767465 | Validation loss 33.349823 | Validation R2 -1.716795
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([ 5.6753,  9.1968,  9.1520,  9.1070,  9.0680, 12.3688, 12.3259, 12.2829,
        12.2460, 15.6801, 15.6373, 15.5945, 15.5579, 18.8876, 18.8448, 18.8021,
        18.7654, 22.0656, 22.0229, 21.9801, 21.9435, 25.1256, 25.0829, 25.0402,
        25.0036, 28.1739, 28.1312, 28.0886, 28.0520, 31.1455, 31.1029, 31.0603,
        31.0238, 34.1763, 34.1337, 34.0912, 34.0547, 37.1030, 37.0544, 37.0118,
        40.1939, 40.1514, 40.1089, 40.0725, 43.2250, 43.1825, 43.1401, 43.1036,
        46.1381, 46.0957, 46.0532, 46.0168, 48.9333, 48.8989, 48.8121, 51.7009,
        51.6585, 51.6222, 54.7601, 54.6392, 57.7422, 57.6999, 57.6637],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0003 | Training loss 25.064499 | Training R2 -0.700776 | Validation loss 33.287090 | Validation R2 -1.706584
        Best loss 32.346756 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.63it/s]
tensor([11.9925, 16.1087, 15.6565, 14.7926, 18.7813, 18.1950, 17.1649],
       grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517])

        Epoch 0004 | Training loss 19.580549 | Training R2 -0.037956 | Validation loss 22.115347 | Validation R2 -0.194696
        Best loss 22.115347 | Best epoch 0004

100%|########################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([11.7457, 16.1828, 15.2492], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0005 | Training loss 17.637089 | Training R2 0.157863 | Validation loss 18.753033 | Validation R2 0.140961
        Best loss 18.753033 | Best epoch 0005

100%|########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([18.9408, 25.6120, 24.2652, 21.7064, 27.7522, 26.0064, 22.9544, 28.8805,
        26.7267, 22.9661], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0006 | Training loss 17.212334 | Training R2 0.197937 | Validation loss 18.404135 | Validation R2 0.172628
        Best loss 18.404135 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.60it/s]
tensor([ 7.4809, 16.4973, 14.5521, 12.8453, 11.0989, 10.8038, 14.5344, 11.6942,
         9.5260,  9.1614], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530])

        Epoch 0007 | Training loss 18.241096 | Training R2 0.099195 | Validation loss 21.649376 | Validation R2 -0.144882
        Best loss 18.404135 | Best epoch 0006

100%|########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([21.2631, 37.7968, 34.6909, 28.8175, 35.9441, 28.1752, 40.1245, 34.2910,
        23.3075, 27.6585, 19.4056, 23.0779, 19.8806, 24.1141, 21.9171],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836, 23.7820,  3.2723, 61.1610, 20.1800])

        Epoch 0008 | Training loss 15.880821 | Training R2 0.317229 | Validation loss 17.267464 | Validation R2 0.271672
        Best loss 17.267464 | Best epoch 0008

100%|########################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([29.5514, 33.9478, 33.5019, 33.0550, 31.7080, 36.2872, 34.6281, 32.9590,
        35.4917, 33.4942, 37.8410, 33.2047, 37.4423, 32.1499, 36.2251, 30.2793,
        34.2453, 27.6422, 31.5599, 24.2538, 28.0946, 21.8433, 24.2154],
       grad_fn=<IndexBackward0>)
tensor([66.9750, 34.8300, 30.4850, 27.1220, 19.3810, 59.4210, 39.4690, 28.2220,
        45.4640, 32.5130, 71.1690, 34.2430, 72.7160, 35.0360, 72.9860, 35.1970,
        73.1260, 35.2700, 73.7120, 35.5420, 73.9550, 35.6660, 66.9750])

        Epoch 0009 | Training loss 15.588125 | Training R2 0.342165 | Validation loss 17.531309 | Validation R2 0.249244
        Best loss 17.267464 | Best epoch 0008

100%|########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([22.3988, 44.0035, 38.3123, 27.5719, 42.2598, 33.7127, 17.9093, 31.7069,
        21.5951, 15.1084, 21.6086, 18.1968, 14.7075, 19.6320, 17.6338, 14.6714,
        18.9939, 17.1625, 14.7096, 18.3896, 16.8863, 14.2772, 17.6625, 16.8937,
        14.1760, 16.9282, 15.6259, 13.6606, 16.4278, 15.1709],
       grad_fn=<IndexBackward0>)
tensor([22.8850, 73.4140, 23.4880,  3.5482, 76.4500, 24.6180,  3.7189, 76.3100,
        24.5840,  3.7138, 76.0510, 21.1850,  3.7013, 75.8210, 24.4220,  3.6893,
        74.9130, 24.1510,  3.6483, 73.3630, 23.6320,  3.5700, 72.1350, 23.2310,
         3.5094, 70.4750, 19.6300,  3.4295, 70.9820, 22.8850])

        Epoch 0010 | Training loss 15.053199 | Training R2 0.386539 | Validation loss 16.905653 | Validation R2 0.301874
```

```
        Best loss 16.905653 | Best epoch 0010

100%|########################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([18.1234, 47.1816, 39.9245], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0011 | Training loss 14.768456 | Training R2 0.409528 | Validation loss 16.615559 | Validation R2 0.325627
        Best loss 16.615559 | Best epoch 0011

100%|########################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([11.6720, 32.8382, 24.0419,  7.9924, 23.3818, 12.4458,  8.1120, 14.4407,
        11.5844,  8.4578], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0790,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225])

        Epoch 0012 | Training loss 14.076530 | Training R2 0.463561 | Validation loss 15.982780 | Validation R2 0.376014
        Best loss 15.982780 | Best epoch 0012

100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([15.4169, 37.7438, 26.4691,  7.0804, 27.0034, 15.1891],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0013 | Training loss 13.712152 | Training R2 0.490973 | Validation loss 15.644684 | Validation R2 0.402134
        Best loss 15.644684 | Best epoch 0013

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([12.0577, 36.3803, 23.6637, 11.4284,  3.9892, 24.7131, 13.2179,  7.2145,
         3.9259, 17.6060, 11.4485,  7.1599,  4.1087, 14.8795, 10.1405,  7.4436,
         5.7456, 12.6350, 10.5755,  8.8864,  7.3162, 13.0429, 11.6113,  9.6312,
         8.1763, 13.7002, 12.1540, 10.3492,  8.4799, 14.0624, 12.3707],
       grad_fn=<IndexBackward0>)
tensor([15.8670, 48.0290, 15.0320,  5.2611,  2.1393, 49.5140, 15.6140,  5.4648,
         2.2222, 49.5850, 15.6390,  5.4735,  2.2257, 49.6100, 15.6440,  5.4753,
         2.2264, 49.5890, 15.6410,  5.4740,  2.2259, 49.5930, 15.6410,  4.7118,
         2.2260, 49.5930, 15.6410,  5.4742,  2.2260, 50.3130, 15.8670])

        Epoch 0014 | Training loss 13.242213 | Training R2 0.525266 | Validation loss 15.322500 | Validation R2 0.426506
        Best loss 15.322500 | Best epoch 0014

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([ 5.4798, 30.7803, 14.7806,  2.5093, -1.7086,  8.5024,  1.9989, -1.6791],
       grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866])

        Epoch 0015 | Training loss 12.924088 | Training R2 0.547802 | Validation loss 14.716954 | Validation R2 0.470939
        Best loss 14.716954 | Best epoch 0015

100%|########################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([15.6168, 55.2221, 16.2939,  8.2661, 24.2689], grad_fn=<IndexBackward0>)
tensor([16.1690, 59.8340,  5.3050,  1.4892, 16.1690])

        Epoch 0016 | Training loss 11.898344 | Training R2 0.616732 | Validation loss 14.322660 | Validation R2 0.498908
        Best loss 14.322660 | Best epoch 0016

100%|########################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([12.7216, 59.7177, 25.1669,  4.2772, 34.5799, 21.0603,  9.3780,  3.6991,
        31.5247, 18.5450,  8.8795,  3.1359, 25.5747, 15.5161,  5.9220],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018,
        65.7810, 20.9510,  4.9462,  1.6753, 64.1100, 17.0690,  4.0299])

        Epoch 0017 | Training loss 11.401729 | Training R2 0.648058 | Validation loss 13.213898 | Validation R2 0.573487
        Best loss 13.213898 | Best epoch 0017

100%|########################################| 672/672 [01:32<00:00,  7.30it/s]
tensor([ 2.9063, 32.5171, 27.8092, 23.1816, 13.6546,  9.5199,  5.4563,  2.9917,
         0.8526, 27.3170, 15.6950,  7.0380,  3.1720, 24.6298, 14.8523,  8.5628,
         4.3510, 22.1035, 15.0576,  8.9973,  5.4540, 22.2026, 13.7354,  9.1169,
         6.3164, 22.1408, 14.2489,  9.6895,  7.1869, 21.7399, 14.4235, 10.2883,
         8.0124, 21.3545, 11.1481,  8.8666, 20.7642, 15.1376, 11.6578,  9.4312,
        20.2414, 15.3670, 12.0332, 10.2129, 21.1668, 16.4321, 13.0078, 10.8106,
        21.6568, 17.0286, 13.6380, 11.4462, 22.2054, 17.6234, 14.2651, 12.1728,
        18.4076, 15.0337], grad_fn=<IndexBackward0>)
tensor([ 2.7419, 28.6490, 21.3580, 16.8180,  8.0564,  4.9078,  2.5526,  1.5643,
         0.9587, 44.6470,  8.7898,  2.7858,  1.0463, 43.9280,  8.6592,  2.7445,
         1.0308, 44.7080,  8.8094,  2.7920,  1.0487, 45.3180,  7.5611,  2.8303,
         1.0630, 45.7270,  9.0111,  2.8560,  1.0727, 45.7350,  9.0137,  2.8568,
         1.0730, 46.3300,  2.8935,  1.0868, 44.3590,  8.7473,  2.7724,  1.0413,
        31.3930,  7.5594,  2.4035,  1.0628, 43.9420,  8.6636,  2.7459,  1.0313,
        43.7170,  8.6165,  2.7309,  1.0257, 43.3150,  8.5378,  2.7060,  1.0163,
         8.6510,  2.7419])

        Epoch 0018 | Training loss 10.813417 | Training R2 0.683441 | Validation loss 13.203379 | Validation R2 0.574166
        Best loss 13.203379 | Best epoch 0018

100%|########################################| 672/672 [01:32<00:00,  7.23it/s]
tensor([ 9.7498, 40.5504, 13.2881,  0.8898, 25.9407, 14.4120,  2.2655,  1.0768,
        24.7947, 14.0786,  1.6502], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568])

        Epoch 0019 | Training loss 10.473630 | Training R2 0.703023 | Validation loss 13.268398 | Validation R2 0.569962
        Best loss 13.203379 | Best epoch 0018

100%|########################################| 672/672 [01:34<00:00,  7.07it/s]
tensor([ 2.5559, 19.4985,  2.8311, 33.7559, 17.7553,  2.5439],
       grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742])

        Epoch 0020 | Training loss 9.496670 | Training R2 0.755842 | Validation loss 10.343183 | Validation R2 0.738677
        Best loss 10.343183 | Best epoch 0020

100%|########################################| 672/672 [01:38<00:00,  6.80it/s]
tensor([ 6.5408, 27.2245, 21.7968, 17.0160, 14.4693,  9.4895, 26.6533, 19.8093,
        14.0566, 29.3762, 22.2869, 16.0390, 30.4389, 16.7182, 30.6311, 16.9595,
        30.6151, 17.0785, 30.7607, 17.0520, 30.7647, 16.8004, 30.8296, 16.6525,
        30.7940, 16.4834, 27.5907, 16.3012, 30.4290, 16.1035, 30.0555, 15.9718,
        29.7875, 15.9149, 29.5319, 15.9032, 15.8856, 26.1478, 15.8869, 28.9241,
        15.8869, 28.7300, 15.8838, 28.5423, 15.8782, 28.2471, 15.7892, 28.3878,
        15.8788, 28.1359, 23.1418], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0021 | Training loss 7.951676 | Training R2 0.828823 | Validation loss 8.662682 | Validation R2 0.816695
        Best loss 8.662682 | Best epoch 0021

100%|########################################| 672/672 [01:46<00:00,  6.31it/s]
tensor([ 5.0714, 41.2239, 10.6933,  1.8153, -1.6648, 32.1178, 11.6598,  2.8483],
       grad_fn=<IndexBackward0>)
tensor([ 2.2708, 40.9840,  9.4533,  2.2722,  0.6695, 40.8030,  9.4476,  2.2708])

        Epoch 0022 | Training loss 7.609004 | Training R2 0.843258 | Validation loss 8.749406 | Validation R2 0.813006
        Best loss 8.662682 | Best epoch 0021

100%|########################################| 672/672 [02:05<00:00,  5.36it/s]
tensor([ 7.4991, 41.7259, 10.5250,  2.0759, -0.8212, -0.1132],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724])

        Epoch 0023 | Training loss 6.876002 | Training R2 0.872003 | Validation loss 6.808918 | Validation R2 0.886753
        Best loss 6.808918 | Best epoch 0023

100%|########################################| 672/672 [02:24<00:00,  4.66it/s]
tensor([10.0532, 11.7258,  3.9000, 25.9815, 11.5955,  4.2005, 24.3615, 10.3238,
         4.2589], grad_fn=<IndexBackward0>)
tensor([16.2540, 16.8150,  3.7307, 46.7120, 18.2510,  4.0494, 39.1610, 16.6890,
         4.1575])

        Epoch 0024 | Training loss 6.344456 | Training R2 0.891027 | Validation loss 6.287634 | Validation R2 0.903429
        Best loss 6.287634 | Best epoch 0024

100%|########################################| 672/672 [02:28<00:00,  4.53it/s]
tensor([ 1.6894, 23.4610,  3.5930, -1.5898, -2.5777, 30.9283,  8.1172,  1.3945,
        -1.0457], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900])

        Epoch 0025 | Training loss 7.193916 | Training R2 0.859893 | Validation loss 8.765650 | Validation R2 0.812311
        Best loss 6.287634 | Best epoch 0024

100%|########################################| 672/672 [02:31<00:00,  4.45it/s]
tensor([ 8.8472, 41.0249,  8.3407,  2.1899, 36.6626, 12.1595],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0026 | Training loss 6.314091 | Training R2 0.892068 | Validation loss 7.142266 | Validation R2 0.875393
        Best loss 6.287634 | Best epoch 0024

100%|########################################| 672/672 [02:34<00:00,  4.34it/s]
tensor([ 8.5633, 52.2498,  1.5635, 17.5187,  1.9039, 16.5124,  1.4483],
       grad_fn=<IndexBackward0>)
tensor([ 5.0480, 57.3470,  1.4345, 18.1510,  1.4741, 17.6580,  1.4340])

        Epoch 0027 | Training loss 6.055744 | Training R2 0.900719 | Validation loss 5.718658 | Validation R2 0.920116
        Best loss 5.718658 | Best epoch 0027

100%|########################################| 672/672 [02:36<00:00,  4.29it/s]
tensor([ 7.0780, 42.2500, 11.1324,  3.1023,  1.2874,  2.6817, 21.2856,  6.6037,
         3.4198], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0028 | Training loss 6.592818 | Training R2 0.882328 | Validation loss 7.770147 | Validation R2 0.852522
```

```
        Best loss 5.718658 | Best epoch 0027

100%|########################################| 672/672 [02:36<00:00,  4.30it/s]
tensor([ 3.7971, 35.3375,  8.4819,  1.6825, -0.3244, -0.4051, 13.2231,  2.0788,
         0.1861,  0.0965, 12.3868,  2.4895,  0.1087,  0.0419],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0029 | Training loss 5.998502 | Training R2 0.902587 | Validation loss 5.604497 | Validation R2 0.923274
        Best loss 5.604497 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 2 --model 4 --save fold_2 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([2.1999, 5.6524, 5.8418, 6.1936, 9.4868, 9.8432],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521])

        Epoch 0001 | Training loss 24.587435 | Training R2 -0.636649 | Validation loss 29.936550 | Validation R2 -1.189140
        Best loss 29.936550 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([ 4.9043,  8.9507,  9.0836,  9.2166,  9.3305, 13.3845, 13.5179, 13.6512,
        13.7654, 17.8186, 17.9522, 18.0858], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243, 63.0070, 16.7890,  4.7756])

        Epoch 0002 | Training loss 25.483650 | Training R2 -0.758136 | Validation loss 33.067993 | Validation R2 -1.671072
        Best loss 29.936550 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 7.6014, 11.0011, 11.0285], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0003 | Training loss 24.522160 | Training R2 -0.627971 | Validation loss 32.016544 | Validation R2 -1.503911
        Best loss 29.936550 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([ 7.3291, 10.1608, 10.0233,  9.8829], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.401255 | Training R2 -0.358544 | Validation loss 28.629280 | Validation R2 -1.002123
        Best loss 28.629280 | Best epoch 0004

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([14.4474, 19.8099, 19.4276, 18.6136, 23.0821, 21.7736, 26.9981, 26.1418,
        24.3684, 28.5206, 26.5152], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836])

        Epoch 0005 | Training loss 19.169922 | Training R2 0.005122 | Validation loss 21.290998 | Validation R2 -0.107291
        Best loss 21.290998 | Best epoch 0005

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([12.2309, 18.9201, 18.0805, 16.3241, 20.7797, 18.8313, 22.8460, 20.6343,
        24.4485, 21.9717], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0006 | Training loss 19.678331 | Training R2 -0.048349 | Validation loss 22.492300 | Validation R2 -0.235770
        Best loss 21.290998 | Best epoch 0005

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 9.0321, 16.7148, 15.5704, 14.4203], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0007 | Training loss 18.438383 | Training R2 0.079604 | Validation loss 20.871935 | Validation R2 -0.064132
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 0.2794,  0.7751,  0.5484, -0.3596, -1.0415, -1.9520, -2.6358, -3.3204,
        -2.3768, -4.0057, -5.6395], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0008 | Training loss 20.370321 | Training R2 -0.123375 | Validation loss 23.957869 | Validation R2 -0.402059
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([17.7417, 27.3907, 25.9303], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0009 | Training loss 19.084763 | Training R2 0.013942 | Validation loss 21.900980 | Validation R2 -0.171647
        Best loss 20.871935 | Best epoch 0007

100%|########################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([17.3056, 25.6101, 24.2517, 20.7280, 26.5591, 24.9605, 21.8946, 26.8496,
        25.2540, 22.2393], grad_fn=<IndexBackward0>)
tensor([17.8830, 55.3190, 16.9870,  2.1271, 56.8470, 17.5230,  2.1942, 57.7130,
        17.7900,  2.2277])

        Epoch 0010 | Training loss 17.859404 | Training R2 0.136499 | Validation loss 20.114540 | Validation R2 0.011697
        Best loss 20.114540 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 8.7530, 19.8132, 16.8510, 16.2882, 22.7456, 19.5403, 19.2723],
       grad_fn=<IndexBackward0>)
tensor([ 9.2660, 25.5950,  5.0055,  3.7205, 26.2690,  4.4291,  3.8185])

        Epoch 0011 | Training loss 18.237335 | Training R2 0.099566 | Validation loss 20.373814 | Validation R2 -0.013945
        Best loss 20.114540 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 9.9975, 15.6876, 13.4450, 11.2903, 17.1275, 15.1765, 11.2384],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727])

        Epoch 0012 | Training loss 17.548340 | Training R2 0.166316 | Validation loss 19.443098 | Validation R2 0.076577
        Best loss 19.443098 | Best epoch 0012

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 9.9177, 18.4395, 17.9721, 17.5216, 14.3823, 12.5939, 11.2551,  9.9186,
        16.4753, 13.0464], grad_fn=<IndexBackward0>)
tensor([ 4.1835, 35.5470, 29.2780, 24.3620,  6.9018,  3.3599,  1.9581,  1.1412,
        14.7460,  4.1835])

        Epoch 0013 | Training loss 17.206947 | Training R2 0.198439 | Validation loss 19.141432 | Validation R2 0.105009
        Best loss 19.141432 | Best epoch 0013

100%|########################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([12.4364, 27.2565, 23.2694, 19.6116, 16.4919, 29.9886, 27.1892, 23.8359,
        20.2824], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243])

        Epoch 0014 | Training loss 17.306837 | Training R2 0.189105 | Validation loss 19.362793 | Validation R2 0.084189
        Best loss 19.141432 | Best epoch 0013

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([ 9.0598, 20.0499, 19.4907, 18.9320, 17.8166, 16.1479, 12.2752, 10.0752,
         8.9788, 18.8787, 14.2877, 10.3545,  8.6562, 18.4221, 14.3182, 10.7028,
         9.1701], grad_fn=<IndexBackward0>)
tensor([ 1.7285, 64.0430, 33.8580, 27.3170, 18.5670, 10.6030,  2.8810,  1.3684,
         0.9431, 27.6900,  6.1533,  1.6721,  0.9567, 23.0690,  6.2359,  1.6946,
         0.9695])

        Epoch 0015 | Training loss 16.755896 | Training R2 0.239911 | Validation loss 19.031542 | Validation R2 0.115256
        Best loss 19.031542 | Best epoch 0015

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([  0.9582,   1.0904,   0.4565,  -1.8299,  -3.4424,  -5.5529,  -7.1404,
         -8.7248,  -7.3052, -10.9318, -14.4289], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0016 | Training loss 16.645119 | Training R2 0.249928 | Validation loss 18.393700 | Validation R2 0.173566
        Best loss 18.393700 | Best epoch 0016

100%|########################################| 672/672 [01:34<00:00,  7.14it/s]
tensor([ 6.8242, 20.9803, 15.5757, 10.6441,  6.5071, 20.2602, 15.3891, 10.3295,
         6.6992, 19.2614, 16.2280, 12.1368,  8.1876], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581])

        Epoch 0017 | Training loss 16.093096 | Training R2 0.298854 | Validation loss 17.970434 | Validation R2 0.211163
        Best loss 17.970434 | Best epoch 0017

100%|########################################| 672/672 [01:38<00:00,  6.82it/s]
tensor([12.8932, 35.1585, 29.2565, 17.6236, 35.2379, 31.1231, 21.2395],
       grad_fn=<IndexBackward0>)
```

```
tensor([ 3.8765, 62.3080, 16.2100,  1.3937, 63.5960, 16.5530,  1.4231])

        Epoch 0018 | Training loss 15.311383 | Training R2 0.365315 | Validation loss 16.984724 | Validation R2 0.295328
        Best loss 16.984724 | Best epoch 0018

100%|########################################| 672/672 [01:49<00:00,  6.14it/s]
tensor([16.5482, 29.7475, 28.0376], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0019 | Training loss 14.230635 | Training R2 0.451751 | Validation loss 15.854136 | Validation R2 0.386019
        Best loss 15.854136 | Best epoch 0019

100%|########################################| 672/672 [02:02<00:00,  5.47it/s]
tensor([19.7466, 42.1145, 30.2606, 14.1118, 37.6893, 25.5962, 11.4744, 34.7414,
        11.2551, 33.2510, 23.2312, 11.2077, 33.0895, 23.2144, 11.2046, 32.8959,
        23.1463, 11.2140, 32.9500, 23.3397, 11.3844, 32.9221, 23.4265, 11.5103,
        23.5826, 11.6663, 32.9310, 23.6521, 11.7840, 32.9144, 23.7639],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0020 | Training loss 12.025496 | Training R2 0.608497 | Validation loss 13.721763 | Validation R2 0.540072
        Best loss 13.721763 | Best epoch 0020

100%|########################################| 672/672 [02:25<00:00,  4.62it/s]
tensor([11.1434, 49.1650, 25.8507, 12.7483], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0021 | Training loss 12.230107 | Training R2 0.595061 | Validation loss 13.446256 | Validation R2 0.558356
        Best loss 13.446256 | Best epoch 0021

100%|########################################| 672/672 [02:41<00:00,  4.16it/s]
tensor([ 7.8498, 35.5636, 31.8140, 27.4297, 23.8189, 15.3497, 39.8910, 28.7233,
        18.5893, 41.4949, 30.8928, 19.8995, 41.8754, 38.6326, 20.1299, 38.6822,
        20.5340, 38.5935, 21.5521], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590])

        Epoch 0022 | Training loss 9.790716 | Training R2 0.740488 | Validation loss 12.751149 | Validation R2 0.602837
        Best loss 12.751149 | Best epoch 0022

100%|########################################| 672/672 [02:38<00:00,  4.23it/s]
tensor([14.1666, 61.5551, 29.6613,  8.8076, 58.5753, 24.2845,  8.8832],
       grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781])

        Epoch 0023 | Training loss 8.497423 | Training R2 0.804519 | Validation loss 10.855521 | Validation R2 0.712147
        Best loss 10.855521 | Best epoch 0023

100%|########################################| 672/672 [02:47<00:00,  4.02it/s]
tensor([15.8495, 61.9667, 28.1483, 10.4488], grad_fn=<IndexBackward0>)
tensor([18.4370, 63.6710, 21.1850,  2.2930])

        Epoch 0024 | Training loss 7.026572 | Training R2 0.866335 | Validation loss 7.219308 | Validation R2 0.872690
        Best loss 7.219308 | Best epoch 0024

100%|########################################| 672/672 [03:04<00:00,  3.64it/s]
tensor([15.0177, 53.2453, 22.2480, 13.1297, 52.0899, 24.2600],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])

        Epoch 0025 | Training loss 22.096283 | Training R2 -0.321805 | Validation loss 31.622337 | Validation R2 -1.442631
        Best loss 7.219308 | Best epoch 0024

100%|########################################| 672/672 [03:00<00:00,  3.72it/s]
tensor([ 9.0573, 64.0458, 19.9370,  7.2607,  4.3328, 59.8810, 18.9035,  3.8537],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0026 | Training loss 6.403774 | Training R2 0.888980 | Validation loss 6.044273 | Validation R2 0.910760
        Best loss 6.044273 | Best epoch 0026

100%|########################################| 672/672 [02:59<00:00,  3.75it/s]
tensor([ 6.9223, 61.5160, 18.7082,  3.0362, 18.1905,  2.9401, 18.2441,  2.8033],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559])

        Epoch 0027 | Training loss 6.205529 | Training R2 0.895747 | Validation loss 6.115032 | Validation R2 0.908659
        Best loss 6.044273 | Best epoch 0026

100%|########################################| 672/672 [02:58<00:00,  3.76it/s]
tensor([ 6.6950, 60.9784, 50.3774, 41.8519, 28.7659, 16.2084,  8.8678,  3.7320,
         2.6390], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0028 | Training loss 6.358976 | Training R2 0.890528 | Validation loss 5.888662 | Validation R2 0.915296
        Best loss 5.888662 | Best epoch 0028

100%|########################################| 672/672 [02:56<00:00,  3.80it/s]
tensor([ 5.4355, 52.7556, 12.8180,  2.5391], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0029 | Training loss 6.320073 | Training R2 0.891863 | Validation loss 5.790334 | Validation R2 0.918101
        Best loss 5.790334 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 2 --model 5 --save fold_2 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([ 2.8724,  6.5957,  6.8080,  6.9899,  7.2021, 10.7213, 10.9348, 11.3314,
        14.8272, 15.0422, 15.1036, 15.4413, 18.9374, 19.1537, 19.5554, 23.0516,
        23.2693, 23.6736, 27.3578, 27.6082, 27.7960, 30.7728, 30.9930, 31.2133],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666,
        61.4260, 21.6510, 16.6580,  3.9438, 61.4060, 21.6430,  3.9424, 61.4240,
        21.6460,  3.9429, 24.6850,  8.6517,  3.9430, 52.7130, 18.6040,  7.4356])

        Epoch 0001 | Training loss 25.439198 | Training R2 -0.752008 | Validation loss 31.925747 | Validation R2 -1.489729
        Best loss 31.925747 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 3.2931,  5.3593,  5.3786,  5.3980,  5.4173,  5.4752,  7.2988,  7.3569,
         7.4149,  9.1766,  9.2347,  9.2928, 11.0515, 11.1676, 12.9117, 13.0278,
        14.7861, 14.9023, 16.6606, 16.7768, 18.5066, 18.6228, 20.3668, 20.4830,
        22.2271, 22.3433, 24.1067, 24.2035, 25.9476, 26.0638, 27.7936, 27.9099,
        29.6397, 29.7559, 31.4857, 31.6020, 33.4481, 35.1973, 35.2942, 37.0240,
        37.1403, 38.8701, 38.9864, 40.7162, 40.8325, 42.5338, 42.6501, 44.3800,
        44.4963, 46.1862, 46.2250], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0002 | Training loss 26.376934 | Training R2 -0.883553 | Validation loss 34.834122 | Validation R2 -1.964010
        Best loss 31.925747 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 7.8250, 11.8784, 11.8799, 11.8814, 11.8873, 11.8917, 11.8975, 11.9019,
        11.9062, 15.7652, 15.7763, 15.7875], grad_fn=<IndexBackward0>)
tensor([ 2.8854, 42.8980, 34.5060, 27.9840, 12.2340,  6.5823,  2.8806,  1.5499,
         0.8339, 54.9410, 12.2540,  2.8854])

        Epoch 0003 | Training loss 24.805820 | Training R2 -0.665852 | Validation loss 32.632885 | Validation R2 -1.601243
        Best loss 31.925747 | Best epoch 0001

100%|########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 8.7386, 11.7069, 11.5418, 11.3754, 11.2797, 11.2316, 13.9237, 13.7604,
        13.6669, 13.6202, 16.3320, 16.2147, 16.1207, 16.0738],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8004,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0004 | Training loss 22.594074 | Training R2 -0.382033 | Validation loss 29.154833 | Validation R2 -1.076304
        Best loss 29.154833 | Best epoch 0004

100%|########################################| 672/672 [01:29<00:00,  7.53it/s]
tensor([13.8576, 17.9291, 17.4015, 16.8603], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0005 | Training loss 19.321512 | Training R2 -0.010675 | Validation loss 21.662233 | Validation R2 -0.146242
        Best loss 21.662233 | Best epoch 0005

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([11.5918, 16.2894, 16.0552], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])
```

```
        Epoch 0006 | Training loss 18.806362 | Training R2 0.042500 | Validation loss 20.810762 | Validation R2 -0.057903
        Best loss 20.810762 | Best epoch 0006

100%|##########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([13.7967, 24.9147, 23.5840, 22.4126, 21.0541, 27.8658, 26.2462, 23.2119],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0007 | Training loss 18.502975 | Training R2 0.073144 | Validation loss 20.257120 | Validation R2 -0.002364
        Best loss 20.257120 | Best epoch 0007

100%|##########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 7.3947, 16.2876, 14.5021], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0008 | Training loss 17.884424 | Training R2 0.134077 | Validation loss 19.712755 | Validation R2 0.050785
        Best loss 19.712755 | Best epoch 0008

100%|##########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 7.4039, 16.9333, 14.2522], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0009 | Training loss 18.018396 | Training R2 0.121056 | Validation loss 20.877218 | Validation R2 -0.064670
        Best loss 19.712755 | Best epoch 0008

100%|##########################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([0.6249, 7.8101, 7.3241, 3.8194, 1.0698], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0010 | Training loss 17.464170 | Training R2 0.174295 | Validation loss 20.522924 | Validation R2 -0.028841
        Best loss 19.712755 | Best epoch 0008

100%|##########################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 9.3226, 15.8665,  8.5315, 13.2728,  7.9733], grad_fn=<IndexBackward0>)
tensor([15.8300, 13.0430,  1.2608, 15.9120,  1.2850])

        Epoch 0011 | Training loss 15.910845 | Training R2 0.314645 | Validation loss 18.198824 | Validation R2 0.190985
        Best loss 18.198824 | Best epoch 0011

100%|##########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 4.3449, 16.5067], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0012 | Training loss 15.860810 | Training R2 0.318949 | Validation loss 18.750023 | Validation R2 0.141237
        Best loss 18.198824 | Best epoch 0011

100%|##########################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([ 8.7084, 25.3828, 17.3558,  9.8191,  3.7226,  1.3463, 10.4619,  6.1137,
         2.9816, 10.1290,  7.5545,  4.8109,  4.4536], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0013 | Training loss 13.904661 | Training R2 0.476580 | Validation loss 15.886896 | Validation R2 0.383479
        Best loss 15.886896 | Best epoch 0013

100%|##########################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([ 7.0433, 27.5600, 16.8307,  7.2308,  0.1864,  9.9691,  3.3722, -0.6687,
         7.9056,  3.2674, -0.1207], grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866,
        16.0580,  5.2932,  1.7451])

        Epoch 0014 | Training loss 12.929752 | Training R2 0.547405 | Validation loss 15.179044 | Validation R2 0.437194
        Best loss 15.179044 | Best epoch 0014

100%|##########################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([ 7.4332, 30.5729, 16.2396], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0015 | Training loss 12.248608 | Training R2 0.593835 | Validation loss 14.446182 | Validation R2 0.490228
        Best loss 14.446182 | Best epoch 0015

100%|##########################################| 672/672 [01:34<00:00,  7.13it/s]
tensor([ 4.6836,  7.6980,  7.1804, 17.4322, 10.2643,  9.2034, 19.8746, 11.5507,
        10.7448, 13.1053, 12.3932, 20.9605, 14.0527, 22.7131, 18.8298],
       grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462,  3.2262,  2.3463, 25.6730,  2.3549, 30.2890,  8.4665])

        Epoch 0016 | Training loss 11.735577 | Training R2 0.627147 | Validation loss 14.173969 | Validation R2 0.509258
        Best loss 14.173969 | Best epoch 0016

100%|##########################################| 672/672 [01:36<00:00,  6.99it/s]
tensor([11.6500, 60.2137, 25.1021, 10.0511], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0017 | Training loss 10.962422 | Training R2 0.674656 | Validation loss 14.000322 | Validation R2 0.521209
        Best loss 14.000322 | Best epoch 0017

100%|##########################################| 672/672 [01:41<00:00,  6.60it/s]
tensor([ 1.9511, 20.6897,  3.2896, -2.9803, -5.5958, 20.0863,  5.9632, -0.5994,
        -4.8749, 19.8183,  6.0784, -1.1292, -4.3055, 19.2795,  7.1646,  0.7781,
        -3.7093], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6828,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900, 35.4880,  5.5170,  0.8985,  0.1896, 35.4880,  7.1499,  1.5090,
         0.1896])

        Epoch 0018 | Training loss 8.945731 | Training R2 0.783349 | Validation loss 10.094747 | Validation R2 0.751079
        Best loss 10.094747 | Best epoch 0018

100%|##########################################| 672/672 [02:00<00:00,  5.56it/s]
tensor([18.3829, 63.2539, 23.4179,  4.5281, 46.1589, 19.9410,  4.2955, 35.4959,
        16.3430,  3.1342, 26.7132, 12.0767,  3.3039,  2.6298],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775])

        Epoch 0019 | Training loss 8.820597 | Training R2 0.789368 | Validation loss 9.154214 | Validation R2 0.795303
        Best loss 9.154214 | Best epoch 0019

100%|##########################################| 672/672 [02:17<00:00,  4.88it/s]
tensor([ 4.1644, 14.0128, -0.3138, 27.2210, 10.2752, -0.3314, 23.0703,  7.9699,
        -0.3345], grad_fn=<IndexBackward0>)
tensor([ 1.7265, 18.3160,  2.4943, 49.3870, 15.7180,  2.1405, 40.9940, 12.9500,
         1.7635])

        Epoch 0020 | Training loss 7.317793 | Training R2 0.855026 | Validation loss 7.885971 | Validation R2 0.848092
        Best loss 7.885971 | Best epoch 0020

100%|##########################################| 672/672 [02:28<00:00,  4.54it/s]
tensor([ 8.4705, 47.7004, 13.9731,  1.0199, 41.2189, 11.3355,  1.4946, 40.8871,
        13.6375,  2.4164, 39.6342, 12.4571,  3.1625], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0021 | Training loss 7.042254 | Training R2 0.865738 | Validation loss 8.384834 | Validation R2 0.828265
        Best loss 7.885971 | Best epoch 0020

100%|##########################################| 672/672 [02:32<00:00,  4.40it/s]
tensor([ 4.4215, 36.0008,  8.1078,  0.6668, -1.3523, -1.4276, 11.2206, -0.1053,
        -1.8685, -1.9566,  9.4959, -0.7273, -2.5235, -2.5964,  8.4442, -2.1228,
        -3.3086, -3.3706], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307])

        Epoch 0022 | Training loss 9.585545 | Training R2 0.751250 | Validation loss 10.479862 | Validation R2 0.731724
        Best loss 7.885971 | Best epoch 0020

100%|##########################################| 672/672 [02:33<00:00,  4.37it/s]
tensor([ 7.7273, 48.1425, 12.7922,  1.4126, 44.4121, 10.8110,  1.8589, 44.7639,
        13.0078,  1.6967, 44.0305, 10.4389,  1.3453], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0023 | Training loss 6.300526 | Training R2 0.892531 | Validation loss 5.878633 | Validation R2 0.915584
        Best loss 5.878633 | Best epoch 0023

100%|##########################################| 672/672 [02:35<00:00,  4.32it/s]
tensor([ 4.2463, 36.7811,  8.6615,  1.4889, -0.0500, -0.0957, 12.9539,  1.7627,
         0.3970,  0.3455, 12.1383,  1.8436,  0.3857,  0.3445, 11.9547,  1.1080,
         0.2285,  0.1806, 11.7720,  1.7816,  0.1081,  7.4648,  1.6911,  0.0825,
        11.4667,  0.7494, -0.1261, -0.1730,  0.2474, -0.3031, 30.3681,  6.5845,
         0.4806, -0.2833], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307, 10.7730,  2.1190,  0.3304,  6.7693,  2.1190,  0.3304,
        10.7810,  1.6811,  0.4171,  0.3307,  1.0556,  0.3304, 35.8960,  6.7693,
         1.3316,  0.4168])

        Epoch 0024 | Training loss 6.111111 | Training R2 0.898896 | Validation loss 5.680680 | Validation R2 0.921174
        Best loss 5.680680 | Best epoch 0024

100%|##########################################| 672/672 [02:42<00:00,  4.15it/s]
tensor([ 8.8150, 11.5567,  4.6076, 11.2782,  5.0257,  6.5838,  5.3709, 11.5210,
         5.6812, 11.6247,  5.9075, 11.7576,  6.1699, 12.0414,  6.4387, 12.2436],
       grad_fn=<IndexBackward0>)
tensor([14.5460, 14.3260,  2.1336, 15.1440,  2.2555,  7.1526,  2.2158, 14.6630,
         2.1838, 14.4490,  2.1519, 14.3450,  2.1365, 14.4340,  2.1497, 14.5460])

        Epoch 0025 | Training loss 6.472453 | Training R2 0.886586 | Validation loss 7.626081 | Validation R2 0.857940
        Best loss 5.680680 | Best epoch 0024

100%|##########################################| 672/672 [02:58<00:00,  3.77it/s]
tensor([ 1.5432,  6.2264,  4.7043,  3.4637,  1.7148,  0.1873, -0.2482, -0.3312,
        -0.3259], grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0026 | Training loss 6.822579 | Training R2 0.873984 | Validation loss 8.459892 | Validation R2 0.825177
```

```
        Best loss 5.680680 | Best epoch 0024

100%|########################################| 672/672 [02:53<00:00,  3.88it/s]
tensor([12.3268, 41.0046, 31.4636], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0027 | Training loss 6.095839 | Training R2 0.899400 | Validation loss 6.896765 | Validation R2 0.883812
        Best loss 5.680680 | Best epoch 0024

100%|########################################| 672/672 [02:48<00:00,  4.00it/s]
tensor([ 3.3598, 38.0550, 32.1865, 26.7041, 11.2778,  5.3198,  1.1977, -0.6329,
        44.5308, 10.9635,  1.2176], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0028 | Training loss 6.544991 | Training R2 0.884030 | Validation loss 6.196602 | Validation R2 0.906206
        Best loss 5.680680 | Best epoch 0024

100%|########################################| 672/672 [02:45<00:00,  4.07it/s]
tensor([ 5.3302, 57.8313, 14.6693,  3.2426,  1.1091, 15.5492,  4.6520,  2.3154,
        58.9204, 16.3087,  2.9498,  2.4515, 56.6236, 16.2949,  5.9694,  2.6612,
        20.1659,  6.1725,  3.0380, 20.9118,  6.8515,  3.4699],
       grad_fn=<IndexBackward0>)
tensor([ 0.8310, 59.4470, 12.7970,  2.9511,  0.8392, 12.6360,  2.9139,  0.8286,
        58.9270, 12.7180,  1.5640,  0.8341, 56.6760, 12.2320,  3.4784,  0.8022,
        15.3490,  3.5396,  0.8163, 15.6260,  3.6034,  0.8310])

        Epoch 0029 | Training loss 6.115059 | Training R2 0.898765 | Validation loss 7.040408 | Validation R2 0.878922
        Best loss 5.680680 | Best epoch 0024

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 3 --model 1 --save fold_3 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|########################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 2.1615,  4.8593,  5.0546,  5.4167,  7.8210,  8.3762, 10.8642, 11.1145,
        11.2536, 13.7084, 14.0987], grad_fn=<IndexBackward0>)
tensor([ 7.7458, 46.1910, 15.8890,  2.9155, 46.8330,  2.9904, 18.0300,  5.5715,
         2.9028, 17.7490,  2.8574])

        Epoch 0001 | Training loss 25.062193 | Training R2 -0.700463 | Validation loss 31.127050 | Validation R2 -1.366714
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([4.8389, 7.9815, 8.0795, 8.1939], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0002 | Training loss 25.686121 | Training R2 -0.786184 | Validation loss 33.511566 | Validation R2 -1.743212
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([10.7876, 14.7278, 14.7281, 14.7284, 14.7289, 14.7298, 14.7307, 14.7318,
        14.7326], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0003 | Training loss 24.546101 | Training R2 -0.631151 | Validation loss 32.111191 | Validation R2 -1.518737
        Best loss 31.127050 | Best epoch 0001

100%|########################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([3.3280, 8.1569], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6958])

        Epoch 0004 | Training loss 22.813705 | Training R2 -0.409032 | Validation loss 29.552938 | Validation R2 -1.133395
        Best loss 29.552938 | Best epoch 0004

100%|########################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([2.0743, 3.6892, 3.5648, 3.4382, 3.1781, 2.7698, 2.3375, 1.7664, 1.4013],
       grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0005 | Training loss 18.439297 | Training R2 0.079513 | Validation loss 20.436989 | Validation R2 -0.020243
        Best loss 20.436989 | Best epoch 0005

100%|########################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([14.8184, 21.9938, 21.1540, 19.1529, 25.6132, 24.3171, 21.8638, 28.2239,
        26.6049, 23.5441, 29.8066, 27.8578, 24.1761], grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781, 68.7910,
        23.4760,  4.5602, 68.2770, 23.3020,  4.5263])

        Epoch 0006 | Training loss 17.760878 | Training R2 0.146000 | Validation loss 19.276941 | Validation R2 0.092292
        Best loss 19.276941 | Best epoch 0006

100%|########################################| 672/672 [01:31<00:00,  7.37it/s]
tensor([ 7.2685, 17.8126, 17.6222, 17.4313, 16.6626, 16.0806, 15.2971, 14.1049,
        19.7325, 18.0599, 16.3651], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0007 | Training loss 17.224669 | Training R2 0.196787 | Validation loss 18.606171 | Validation R2 0.154363
        Best loss 18.606171 | Best epoch 0007

100%|########################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 8.3480, 18.9609, 17.0796, 13.5076, 19.1425, 16.7568, 12.2467, 17.5037,
        15.0191,  9.3061, 14.1835, 11.0108], grad_fn=<IndexBackward0>)
tensor([ 4.9161, 42.0730,  5.4589, 60.7050, 39.7010,  5.1625,  0.1270, 38.5530,
         6.6617,  0.1233, 37.8370,  4.9161])

        Epoch 0008 | Training loss 16.808960 | Training R2 0.235089 | Validation loss 18.387007 | Validation R2 0.174167
        Best loss 18.387007 | Best epoch 0008

100%|########################################| 672/672 [01:33<00:00,  7.19it/s]
tensor([ 5.5405, 18.0450, 15.2522, 13.2369, 12.8317, 18.4610, 14.6605, 11.4213,
        11.8837, 10.3732, 10.1442, 13.0661, 11.2028,  9.8967,  9.6595],
       grad_fn=<IndexBackward0>)
tensor([ 9.8083, 13.5140,  3.7950,  1.5319,  1.2778, 13.2800,  3.7295,  1.2557,
         3.7290,  1.5053,  1.2555, 13.1880,  3.7035,  1.4950,  1.2470])

        Epoch 0009 | Training loss 16.176075 | Training R2 0.291605 | Validation loss 17.658480 | Validation R2 0.238313
        Best loss 17.658480 | Best epoch 0009

100%|########################################| 672/672 [01:34<00:00,  7.12it/s]
tensor([ 4.4795, 11.8215,  9.0239,  6.1657, 12.2526,  8.1955,  6.0050,  5.2888,
        5.0226], grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625])

        Epoch 0010 | Training loss 15.784349 | Training R2 0.325499 | Validation loss 17.559269 | Validation R2 0.246848
        Best loss 17.559269 | Best epoch 0010

100%|########################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([12.7334, 35.1197, 29.4521, 23.7096, 18.7326, 32.3226, 24.1075],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0011 | Training loss 19.306719 | Training R2 -0.009128 | Validation loss 25.415319 | Validation R2 -0.577833
        Best loss 17.559269 | Best epoch 0010

100%|########################################| 672/672 [01:32<00:00,  7.27it/s]
tensor([32.0389, 42.7443, 41.9388, 41.1327, 39.5190, 37.9050, 47.3776, 44.8538,
        40.7275, 49.5277, 43.8861, 41.0659, 49.2414, 39.0088, 46.8657, 34.8696,
        42.4265, 29.7071, 36.3832, 27.1146, 31.6529, 26.3287, 30.2598, 25.4865],
       grad_fn=<IndexBackward0>)
tensor([58.5520, 41.9580, 32.6790, 27.1470, 20.1960, 15.4500, 55.2420, 32.3270,
        21.5820, 60.6230, 31.3470, 24.0360, 61.8120, 24.6620, 62.3610, 24.9130,
        62.5810, 25.0130, 62.4280, 24.9640, 62.3850, 24.9450, 62.3680, 24.9370])

        Epoch 0012 | Training loss 15.314219 | Training R2 0.365080 | Validation loss 18.021051 | Validation R2 0.206713
        Best loss 17.559269 | Best epoch 0010

100%|########################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 0.5030,  2.0243,  1.2888,  0.5755,  0.0550, -1.1188, -1.4900, -1.7581,
        -1.9126, -2.0494, -1.1390, -1.4614, -1.5448, -1.7284, -1.9236],
       grad_fn=<IndexBackward0>)
tensor([0.1027, 4.3675, 3.3207, 2.6789, 2.2198, 1.1160, 0.6726, 0.3426, 0.2066,
        0.1245, 4.4427, 1.1442, 0.8164, 0.3513, 0.1277])

        Epoch 0013 | Training loss 14.627570 | Training R2 0.420740 | Validation loss 16.876558 | Validation R2 0.304275
        Best loss 16.876558 | Best epoch 0013

 41%|###############7                       | 275/672 [00:37<01:27,  4.52it/s]100%|########################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 8.8011, 44.5529, 42.7156, 40.8827, 31.7829, 26.4018, 19.3116,  9.0496,
        38.4039, 23.2554, 15.9224, 11.0489, 20.7719, 15.0965, 11.2353, 18.4193,
        15.1102, 12.8798, 18.1327, 16.6533, 15.1084, 19.4565, 18.0770, 16.5790,
        18.9628], grad_fn=<IndexBackward0>)
tensor([ 4.2077, 59.4320, 46.9050, 38.1280, 14.2580,  7.9220,  3.6186,  1.1171,
        59.4890, 17.3990,  4.4157,  1.1207, 17.1950,  4.3640,  1.1075, 17.2810,
         4.3856,  1.1130, 16.8630,  5.2057,  1.0861, 16.8560,  4.2779,  1.0857,
         4.2077])

        Epoch 0014 | Training loss 13.552494 | Training R2 0.502758 | Validation loss 15.915753 | Validation R2 0.381237
        Best loss 15.915753 | Best epoch 0014
```

```
100%|##############| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 4.4982, 21.3597,  5.1706], grad_fn=<IndexBackward0>)
tensor([ 4.6703, 20.6660,  3.8425])

        Epoch 0015 | Training loss 13.312044 | Training R2 0.520246 | Validation loss 15.572647 | Validation R2 0.407628
        Best loss 15.572647 | Best epoch 0015

100%|##############| 672/672 [01:34<00:00,  7.12it/s]
tensor([ 5.1438,  8.7150,  8.2335, 17.3058, 10.0088,  9.1330, 17.2026, 10.6696,
        10.4114], grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462])

        Epoch 0016 | Training loss 12.642657 | Training R2 0.567281 | Validation loss 14.518663 | Validation R2 0.485100
        Best loss 14.518663 | Best epoch 0016

100%|##############| 672/672 [01:35<00:00,  7.05it/s]
tensor([ 8.6458, 39.9109, 19.5235,  1.5698, 25.5519, 13.4577,  2.6799],
       grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173])

        Epoch 0017 | Training loss 12.009523 | Training R2 0.609536 | Validation loss 13.955899 | Validation R2 0.524243
        Best loss 13.955899 | Best epoch 0017

100%|##############| 672/672 [01:35<00:00,  7.02it/s]
tensor([16.5268, 53.2245, 25.6311,  4.3723, 32.4923, 17.3056,  3.8944, 25.6408,
        15.9058,  4.0992], grad_fn=<IndexBackward0>)
tensor([12.3700, 69.3770, 19.4920,  2.1362, 68.1120, 16.1970,  2.1042, 46.9250,
        16.8400,  2.1878])

        Epoch 0018 | Training loss 11.491714 | Training R2 0.642481 | Validation loss 14.003984 | Validation R2 0.520958
        Best loss 13.955899 | Best epoch 0017

100%|##############| 672/672 [01:34<00:00,  7.13it/s]
tensor([12.2880, 60.9434, 23.6948,  3.7652, 41.1423, 23.2139,  4.3050, 37.7644,
        21.6612, 10.9115,  4.7921, 33.1801, 17.9587,  9.4201,  4.5785],
       grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370, 62.9420, 16.8690,  6.5668,  3.3492])

        Epoch 0019 | Training loss 10.620493 | Training R2 0.694636 | Validation loss 12.171548 | Validation R2 0.638123
        Best loss 12.171548 | Best epoch 0019

100%|##############| 672/672 [01:35<00:00,  7.00it/s]
tensor([17.7791, 60.7902, 21.8121,  3.3622, 36.1535, 18.7518,  3.8016, 34.5173,
        18.5345,  3.7166], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0020 | Training loss 9.667159 | Training R2 0.746996 | Validation loss 11.243977 | Validation R2 0.691177
        Best loss 11.243977 | Best epoch 0020

100%|##############| 672/672 [01:37<00:00,  6.90it/s]
tensor([ 6.4277, 43.8652, 10.8547,  0.8505], grad_fn=<IndexBackward0>)
tensor([ 1.7780, 53.9210, 16.2500,  5.2152])

        Epoch 0021 | Training loss 9.009152 | Training R2 0.780266 | Validation loss 9.978053 | Validation R2 0.756801
        Best loss 9.978053 | Best epoch 0021

100%|##############| 672/672 [01:38<00:00,  6.79it/s]
tensor([ 7.1529, 44.6963, 12.5524,  2.6736, -0.6076, -1.8314, 12.8853,  3.2542,
         0.2715, -0.8585, 10.7207,  4.6728,  1.5571,  0.3938],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8004,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0022 | Training loss 8.104481 | Training R2 0.822180 | Validation loss 8.888013 | Validation R2 0.807035
        Best loss 8.888013 | Best epoch 0022

100%|##############| 672/672 [01:45<00:00,  6.36it/s]
tensor([ 9.0191, 62.1389,  0.5210, -0.0926,  2.1431], grad_fn=<IndexBackward0>)
tensor([ 2.7853, 66.9550,  2.7495,  2.3342,  2.7853])

        Epoch 0023 | Training loss 8.010061 | Training R2 0.826300 | Validation loss 9.681182 | Validation R2 0.771057
        Best loss 8.888013 | Best epoch 0022

100%|##############| 672/672 [01:57<00:00,  5.70it/s]
tensor([ 3.4122,  6.5380,  0.7621, -1.5433, 25.6093,  7.9584,  1.0656, -0.6848,
        -1.0974,  7.6864,  3.0400, -1.3328, 15.6097,  3.6924, -0.7531, -1.4187,
        17.5918,  4.1631, -0.1998, -1.6550, 11.6587, -1.1651, -2.1033, 22.8726,
         5.6306, -0.3096, -2.2767, 22.2590,  5.2173, -0.8715, -2.5756, 21.4615,
         3.5346, -1.2039, -2.7982, 20.7264,  1.8163, -2.2834],
       grad_fn=<IndexBackward0>)
tensor([ 3.7684, 12.6090,  4.9213,  1.9207, 47.7030, 15.0700,  5.0281,  2.6854,
         1.9625, 15.0820,  8.0548,  1.9640, 29.0970,  9.7026,  3.2372,  2.0224,
        33.9450, 11.2970,  4.4089,  2.0129, 24.7420,  3.7684,  2.0126, 48.9190,
        15.4550,  5.1565,  2.0125, 48.9190, 15.4550,  5.1565,  2.0125, 48.9190,
        13.2120,  5.1565,  2.0125, 48.9190, 11.2950,  3.7684])

        Epoch 0024 | Training loss 7.332561 | Training R2 0.854441 | Validation loss 7.375947 | Validation R2 0.867106
        Best loss 7.375947 | Best epoch 0024

100%|##############| 672/672 [02:20<00:00,  4.79it/s]
tensor([17.5115, 75.5686, 24.1151,  5.0300, 47.8986, 15.6807,  4.7381, 48.6322,
         3.4479, 40.0268, 15.2362], grad_fn=<IndexBackward0>)
tensor([17.5830, 71.0850, 22.2940,  2.9600, 49.2230, 14.1200,  2.9876, 52.3580,
         3.1778, 44.7320, 17.5830])

        Epoch 0025 | Training loss 8.509421 | Training R2 0.803967 | Validation loss 9.115965 | Validation R2 0.797010
        Best loss 7.375947 | Best epoch 0024

100%|##############| 672/672 [02:27<00:00,  4.55it/s]
tensor([ 9.7489, 43.1830, 33.0272, 24.0184, 12.7075,  8.0704,  4.5794,  2.5688,
        37.6630, 14.1537,  6.5239,  4.7297, 40.0373, 15.7862,  7.8193,  6.2941,
        41.6687, 24.4470,  7.7723,  7.5809, 42.2466, 14.8588, 10.3533,  8.6096,
        42.5899, 18.5460, 11.0454,  9.2425, 43.5388, 17.5699, 11.5147,  9.8455,
        44.1187, 19.8935, 11.9677, 10.3997, 44.5415, 20.4890],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385,
        43.0630, 20.8330,  1.9210,  1.3667, 43.0860,  8.8969,  3.7979,  1.3674,
        42.5380, 12.3470,  3.7496,  1.3500, 42.9850, 10.5230,  3.7888,  1.3642,
        43.0840, 12.5050,  3.7977,  1.3674, 43.0840, 12.5050])

        Epoch 0026 | Training loss 7.642862 | Training R2 0.841860 | Validation loss 9.652371 | Validation R2 0.772418
        Best loss 7.375947 | Best epoch 0024

100%|##############| 672/672 [02:28<00:00,  4.51it/s]
tensor([ 8.1295, 16.1995,  3.9024, 38.7570, 16.0048], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0027 | Training loss 6.217919 | Training R2 0.895331 | Validation loss 6.709231 | Validation R2 0.890045
        Best loss 6.709231 | Best epoch 0027

100%|##############| 672/672 [02:32<00:00,  4.41it/s]
tensor([ 2.9591, 16.0822,  0.4870, 41.0720, 13.1148,  0.7645, 43.0557, 15.5036,
         2.9654,  1.1200, 14.4833,  3.8689,  1.5330, 17.2718,  4.1735,  2.0491,
         5.0674,  2.6229,  7.1752,  3.4310, 51.3981,  6.0681,  3.6774,  8.0776,
         4.6272, 41.4533,  7.2080,  4.7518], grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742, 43.9160, 13.4380,
         2.8234,  1.0649, 12.6990,  3.2428,  1.0864, 15.4190,  3.2397,  1.0854,
         3.3101,  1.0273,  4.8677,  1.0228, 53.4230,  3.3111,  1.0275,  4.8942,
         1.0283, 40.7690,  3.8721,  0.9887])

        Epoch 0028 | Training loss 6.286502 | Training R2 0.895715 | Validation loss 7.057861 | Validation R2 0.878321
        Best loss 6.709231 | Best epoch 0027

100%|##############| 672/672 [02:37<00:00,  4.26it/s]
tensor([ 7.6626, 77.2475, 59.0601, 48.7603, 39.5699, 12.5270,  0.4892, -2.0569,
        -3.5056, 59.4931, 14.3282,  1.8468, -1.0112, 59.4113, 14.9668,  2.1448,
        -0.3603, 60.1407, 15.7482,  2.9394,  0.3238], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947, 73.8930, 26.4440, 10.0160,
         5.0069, 74.0470, 26.5260, 10.0480,  5.0226])

        Epoch 0029 | Training loss 5.844729 | Training R2 0.907518 | Validation loss 5.710489 | Validation R2 0.920344
        Best loss 5.710489 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 3 --model 2 --save fold_3 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##############| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 2.8156,  6.4742,  6.6527,  6.8312,  6.9842, 10.4804, 10.6588],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0001 | Training loss 25.589478 | Training R2 -0.772768 | Validation loss 32.346756 | Validation R2 -1.555826
        Best loss 32.346756 | Best epoch 0001

100%|##############| 672/672 [01:32<00:00,  7.27it/s]
tensor([1.9038, 5.0573, 5.0673, 5.1375, 5.1977], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])
```

```
        Epoch 0002 | Training loss 25.551172 | Training R2 -0.767465 | Validation loss 33.349823 | Validation R2 -1.716795
        Best loss 32.346756 | Best epoch 0001

100%|##############| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 5.6753,  9.1968,  9.1520,  9.1070,  9.0680, 12.3688, 12.3259, 12.2829,
        12.2460, 15.6801, 15.6373, 15.5945, 15.5579, 18.8876, 18.8448, 18.8021,
        18.7654, 22.0656, 22.0229, 21.9801, 21.9435, 25.1256, 25.0829, 25.0402,
        25.0036, 28.1739, 28.1312, 28.0886, 28.0520, 31.1455, 31.1029, 31.0603,
        31.0238, 34.1763, 34.1337, 34.0912, 34.0547, 37.1030, 37.0544, 37.0118,
        40.1939, 40.1514, 40.1089, 40.0725, 43.2250, 43.1825, 43.1401, 43.1036,
        46.1381, 46.0957, 46.0532, 46.0168, 48.9333, 48.8909, 48.8121, 51.7009,
        51.6585, 51.6222, 54.7601, 54.6392, 57.7422, 57.6999, 57.6637],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0003 | Training loss 25.064499 | Training R2 -0.700776 | Validation loss 33.287090 | Validation R2 -1.706584
        Best loss 32.346756 | Best epoch 0001

100%|##############| 672/672 [01:34<00:00,  7.12it/s]
tensor([11.9925, 16.1087, 15.6565, 14.7926, 18.7813, 18.1950, 17.1649],
       grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517])

        Epoch 0004 | Training loss 19.580549 | Training R2 -0.037956 | Validation loss 22.115347 | Validation R2 -0.194696
        Best loss 22.115347 | Best epoch 0004

100%|##############| 672/672 [01:32<00:00,  7.30it/s]
tensor([11.7457, 16.1828, 15.2492], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6638])

        Epoch 0005 | Training loss 17.637089 | Training R2 0.157863 | Validation loss 18.753033 | Validation R2 0.140961
        Best loss 18.753033 | Best epoch 0005

100%|##############| 672/672 [01:29<00:00,  7.50it/s]
tensor([18.9408, 25.6120, 24.2652, 21.7064, 27.7522, 26.0064, 22.9544, 28.8805,
        26.7267, 22.9661], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0006 | Training loss 17.212334 | Training R2 0.197937 | Validation loss 18.404135 | Validation R2 0.172628
        Best loss 18.404135 | Best epoch 0006

100%|##############| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 7.4809, 16.4973, 14.5521, 12.8453, 11.0989, 10.8038, 14.5344, 11.6942,
         9.5260,  9.1614], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530])

        Epoch 0007 | Training loss 18.241096 | Training R2 0.099195 | Validation loss 21.649376 | Validation R2 -0.144882
        Best loss 18.404135 | Best epoch 0006

100%|##############| 672/672 [01:28<00:00,  7.61it/s]
tensor([21.2631, 37.7968, 34.6909, 28.8175, 35.9441, 28.1752, 40.1245, 34.2910,
        23.3075, 27.6585, 19.4856, 23.0779, 19.0806, 24.1141, 21.9171],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836, 23.7820,  3.2723, 61.1610, 20.1800])

        Epoch 0008 | Training loss 15.880821 | Training R2 0.317229 | Validation loss 17.267464 | Validation R2 0.271672
        Best loss 17.267464 | Best epoch 0008

100%|##############| 672/672 [01:28<00:00,  7.56it/s]
tensor([29.5514, 33.9478, 33.5019, 33.0550, 31.7080, 36.2872, 34.6281, 32.9590,
        35.4917, 33.4942, 37.8410, 33.2047, 37.4423, 32.1499, 36.2251, 30.2793,
        34.2453, 27.6422, 31.5599, 24.2538, 28.8946, 21.8433, 24.2154],
       grad_fn=<IndexBackward0>)
tensor([66.9750, 34.8300, 30.4850, 27.1220, 19.3810, 59.4210, 39.4690, 28.2220,
        45.4640, 32.5130, 71.1690, 34.2430, 72.7160, 35.0360, 72.9860, 35.1970,
        73.1260, 35.2700, 73.7120, 35.5420, 73.9550, 35.6660, 66.9750])

        Epoch 0009 | Training loss 15.588125 | Training R2 0.342165 | Validation loss 17.531309 | Validation R2 0.249244
        Best loss 17.267464 | Best epoch 0008

100%|##############| 672/672 [01:30<00:00,  7.45it/s]
tensor([22.3988, 44.0035, 38.3123, 27.5719, 42.2598, 33.7127, 17.9093, 31.7069,
        21.5951, 15.1084, 21.6086, 18.1968, 14.7075, 19.6329, 17.6338, 14.6714,
        18.9939, 17.1625, 14.7096, 18.3896, 16.8863, 14.2772, 17.6625, 16.0937,
        14.1760, 16.9282, 15.6259, 13.6606, 16.4278, 15.1709],
       grad_fn=<IndexBackward0>)
tensor([22.8850, 73.4140, 23.4880,  3.5482, 76.4500, 24.6180,  3.7189, 76.3100,
        24.5840,  3.7138, 76.0510, 21.1850,  3.7013, 75.8210, 24.4220,  3.6893,
        74.9130, 24.1510,  3.6483, 73.3630, 23.6320,  3.5700, 72.1350, 23.2310,
         3.5094, 70.4750, 19.6300,  3.4295, 70.9820, 22.8850])

        Epoch 0010 | Training loss 15.053199 | Training R2 0.386539 | Validation loss 16.905653 | Validation R2 0.301874
        Best loss 16.905653 | Best epoch 0010

100%|##############################################################################################################################################################################| 672/672 [01:31<00:00,  7.30it/s]
tensor([18.1234, 47.1816, 39.9245], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0011 | Training loss 14.768456 | Training R2 0.409528 | Validation loss 16.615559 | Validation R2 0.325627
        Best loss 16.615559 | Best epoch 0011

100%|##############################################################################################################################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([11.6720, 32.8382, 24.0419,  7.9924, 23.3818, 12.4458,  8.1120, 14.4407,
        11.5844,  8.4578], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0790,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225])

        Epoch 0012 | Training loss 14.076530 | Training R2 0.463561 | Validation loss 15.982780 | Validation R2 0.376014
        Best loss 15.982780 | Best epoch 0012

100%|##############################################################################################################################################################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([15.4169, 37.7438, 26.4691,  7.0804, 27.0034, 15.1891],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0013 | Training loss 13.712152 | Training R2 0.490973 | Validation loss 15.644684 | Validation R2 0.402134
        Best loss 15.644684 | Best epoch 0013

100%|##############################################################################################################################################################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([12.0577, 36.3803, 23.6637, 11.4284,  3.9892, 24.7131, 13.2179,  7.2145,
         3.9259, 17.6060, 11.4485,  7.1599,  4.1087, 14.8795, 10.1405,  7.4436,
         5.7456, 12.6350, 10.5755,  8.8864,  7.3162, 13.0429, 11.6113,  9.6312,
         8.1763, 13.7002, 12.1540, 10.3492,  8.4799, 14.0624, 12.3707],
       grad_fn=<IndexBackward0>)
tensor([15.8670, 48.0290, 15.8320,  5.2611,  2.1393, 49.5140, 15.6140,  5.4648,
         2.2222, 49.5850, 15.6390,  5.4735,  2.2257, 49.6100, 15.6440,  5.4753,
         2.2264, 49.5890, 15.6410,  5.4740,  2.2259, 49.5930, 15.6410,  4.7118,
         2.2260, 49.5930, 15.6410,  5.4742,  2.2260, 50.3130, 15.8670])

        Epoch 0014 | Training loss 13.242213 | Training R2 0.525266 | Validation loss 15.322500 | Validation R2 0.426506
        Best loss 15.322500 | Best epoch 0014

100%|##############################################################################################################################################################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 5.4798, 30.7803, 14.7806,  2.5093, -1.7086,  8.5024,  1.9989, -1.6791],
       grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866])

        Epoch 0015 | Training loss 12.924088 | Training R2 0.547802 | Validation loss 14.716954 | Validation R2 0.470939
        Best loss 14.716954 | Best epoch 0015

100%|##############################################################################################################################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([15.6168, 55.2221, 16.2939,  8.2661, 24.2689], grad_fn=<IndexBackward0>)
tensor([16.1690, 59.8340,  5.3050,  1.4892, 16.1690])

        Epoch 0016 | Training loss 11.898344 | Training R2 0.616732 | Validation loss 14.322660 | Validation R2 0.498908
        Best loss 14.322660 | Best epoch 0016

100%|##############################################################################################################################################################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([12.7216, 59.7177, 25.1669,  4.2772, 34.5799, 21.0603,  9.3780,  3.6991,
        31.5247, 18.5450,  8.8795,  3.1359, 25.5747, 15.5161,  5.9220],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018,
        65.7810, 20.9510,  4.9462,  1.6753, 64.1100, 17.0690,  4.0299])

        Epoch 0017 | Training loss 11.401729 | Training R2 0.648058 | Validation loss 13.213898 | Validation R2 0.573487
        Best loss 13.213898 | Best epoch 0017

100%|##############################################################################################################################################################################| 672/672 [01:36<00:00,  6.96it/s]
tensor([ 2.9063, 32.5171, 27.8092, 23.1816, 13.6546,  9.5199,  5.4563,  2.9917,
         0.8526, 27.3170, 15.6950,  7.0380,  3.1720, 24.6298, 14.8523,  8.5628,
         4.3510, 22.1035, 15.0576,  8.9973,  5.4540, 22.2026, 13.7354,  9.1169,
         6.3164, 22.1408, 14.2489,  9.6895,  7.1869, 21.7399, 14.4235, 10.2883,
         8.0124, 21.3545, 11.1481,  8.8666, 20.7642, 15.1376, 11.6578,  9.4312,
        20.2414, 15.3670, 12.0332, 10.2129, 21.1668, 16.4321, 13.0078, 10.8106,
        21.6568, 17.0286, 13.6380, 11.4462, 22.2054, 17.6234, 14.2651, 12.1728,
        18.4076, 15.8337], grad_fn=<IndexBackward0>)
tensor([ 2.7419, 28.6490, 21.3580, 16.8180,  8.0564,  4.9078,  2.5526,  1.5643,
         0.9587, 44.6470,  8.7898,  2.7858,  1.0463, 43.9280,  8.6592,  2.7445,
         1.0308, 44.7080,  8.8094,  2.7920,  1.0487, 45.3180,  7.5611,  2.8303,
         1.0630, 45.7270,  9.0111,  2.8560,  1.0727, 45.7350,  9.0137,  2.8568,
         1.0730, 46.3300,  2.8935,  1.0868, 44.3590,  8.7473,  2.7724,  1.0413,
        31.3930,  7.5594,  2.4035,  1.0628, 43.9420,  8.6636,  2.7459,  1.0313,
        43.7170,  8.6165,  2.7309,  1.0257, 43.3150,  8.5378,  2.7060,  1.0163,
         8.6510,  2.7419])

        Epoch 0018 | Training loss 10.813417 | Training R2 0.683441 | Validation loss 13.203379 | Validation R2 0.574166
        Best loss 13.203379 | Best epoch 0018
```

```
100%|##########| 672/672 [01:32<00:00,  7.23it/s]
tensor([ 9.7498, 40.5504, 13.2881,  0.8898, 25.9407, 14.4120,  2.2655,  1.0768,
        24.7947, 14.0786,  1.6502], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568])

        Epoch 0019 | Training loss 10.473630 | Training R2 0.703023 | Validation loss 13.268398 | Validation R2 0.569962
        Best loss 13.203379 | Best epoch 0018

100%|##########| 672/672 [01:37<00:00,  6.90it/s]
tensor([ 2.5559, 19.4985,  2.8311, 33.7559, 17.7553,  2.5439],
       grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742])

        Epoch 0020 | Training loss 9.496670 | Training R2 0.755842 | Validation loss 10.343183 | Validation R2 0.738677
        Best loss 10.343183 | Best epoch 0020

100%|##########| 672/672 [01:43<00:00,  6.52it/s]
tensor([ 6.5408, 27.2245, 21.7968, 17.0160, 14.4693,  9.4895, 26.6533, 19.8093,
        14.0566, 29.3762, 22.2869, 16.0390, 30.4389, 16.7182, 30.6311, 16.9595,
        30.6151, 17.0785, 30.7607, 17.0520, 30.7647, 16.8004, 30.8296, 16.6525,
        30.7940, 16.4834, 27.5907, 16.3012, 30.4290, 16.1035, 30.0555, 15.9718,
        29.7875, 15.9149, 29.5319, 15.9032, 15.8856, 26.1478, 15.8869, 28.9241,
        15.8869, 28.7300, 15.8838, 28.5423, 15.8782, 28.2471, 15.7892, 28.3878,
        15.8788, 28.1359, 23.1418], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0021 | Training loss 7.951676 | Training R2 0.828823 | Validation loss 8.662682 | Validation R2 0.816695
        Best loss 8.662682 | Best epoch 0021

100%|##########| 672/672 [01:49<00:00,  6.14it/s]
tensor([ 5.0714, 41.2239, 10.6933,  1.8153, -1.6648, 32.1178, 11.6598,  2.8483],
       grad_fn=<IndexBackward0>)
tensor([ 2.2708, 40.9040,  9.4533,  2.2722,  0.6695, 40.8030,  9.4476,  2.2708])

        Epoch 0022 | Training loss 7.609004 | Training R2 0.843258 | Validation loss 8.749406 | Validation R2 0.813006
        Best loss 8.662682 | Best epoch 0021

100%|##########| 672/672 [02:05<00:00,  5.37it/s]
tensor([ 7.4991, 41.7259, 10.5250,  2.0759, -0.8212, -0.1132],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724])

        Epoch 0023 | Training loss 6.876002 | Training R2 0.872003 | Validation loss 6.808918 | Validation R2 0.886753
        Best loss 6.808918 | Best epoch 0023

100%|##########| 672/672 [02:26<00:00,  4.60it/s]
tensor([10.0532, 11.7258,  3.9000, 25.9815, 11.5955,  4.2005, 24.3615, 10.3238,
         4.2509], grad_fn=<IndexBackward0>)
tensor([16.2540, 16.8150,  3.7307, 46.7120, 18.2510,  4.0494, 39.1610, 16.6890,
         4.1575])

        Epoch 0024 | Training loss 6.344456 | Training R2 0.891027 | Validation loss 6.287634 | Validation R2 0.903429
        Best loss 6.287634 | Best epoch 0024

100%|##########| 672/672 [02:28<00:00,  4.54it/s]
tensor([ 1.6894, 23.4610,  3.5930, -1.5898, -2.5777, 30.9283,  8.1172,  1.3945,
        -1.0457], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900])

        Epoch 0025 | Training loss 7.193916 | Training R2 0.859893 | Validation loss 8.765650 | Validation R2 0.812311
        Best loss 6.287634 | Best epoch 0024

100%|##########| 672/672 [02:30<00:00,  4.46it/s]
tensor([ 8.8472, 41.0249,  8.3407,  2.1899, 36.6626, 12.1595],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0026 | Training loss 6.314091 | Training R2 0.892068 | Validation loss 7.142266 | Validation R2 0.875393
        Best loss 6.287634 | Best epoch 0024

100%|##########| 672/672 [02:34<00:00,  4.34it/s]
tensor([ 8.5633, 52.2498,  1.5635, 17.5187,  1.9039, 16.5124,  1.4483],
       grad_fn=<IndexBackward0>)
tensor([ 5.0480, 57.3470,  1.4345, 18.1510,  1.4741, 17.6580,  1.4340])

        Epoch 0027 | Training loss 6.055744 | Training R2 0.900719 | Validation loss 5.718658 | Validation R2 0.920116
        Best loss 5.718658 | Best epoch 0027

100%|##########| 672/672 [02:39<00:00,  4.20it/s]
tensor([ 7.0780, 42.2500, 11.1324,  3.1023,  1.2874,  2.6817, 21.2856,  6.6037,
         3.4198], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0028 | Training loss 6.592818 | Training R2 0.882328 | Validation loss 7.770147 | Validation R2 0.852522
        Best loss 5.718658 | Best epoch 0027

100%|##########| 672/672 [02:36<00:00,  4.30it/s]
tensor([ 3.7971, 35.3375,  8.4819,  1.6825, -0.3244, -0.4051, 13.2231,  2.0788,
         0.1861,  0.0965, 12.3060,  2.4895,  0.1087,  0.0419],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.8910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0029 | Training loss 5.998502 | Training R2 0.902587 | Validation loss 5.604497 | Validation R2 0.923274
        Best loss 5.604497 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 3 --model 3 --save fold_3 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########| 672/672 [01:27<00:00,  7.64it/s]
tensor([2.1999, 5.6524, 5.8418, 6.1936, 9.4868, 9.8432],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521])

        Epoch 0001 | Training loss 24.587435 | Training R2 -0.636649 | Validation loss 29.936550 | Validation R2 -1.189140
        Best loss 29.936550 | Best epoch 0001

100%|##########| 672/672 [01:28<00:00,  7.62it/s]
tensor([ 4.9043,  8.9507,  9.0836,  9.2166,  9.3305, 13.3845, 13.5179, 13.6512,
        13.7654, 17.8186, 17.9522, 18.0858], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243, 63.0070, 16.7890,  4.7756])

        Epoch 0002 | Training loss 25.483650 | Training R2 -0.758136 | Validation loss 33.067993 | Validation R2 -1.671072
        Best loss 29.936550 | Best epoch 0001

100%|##########| 672/672 [01:27<00:00,  7.65it/s]
tensor([ 7.6014, 11.0011, 11.0285], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0003 | Training loss 24.522160 | Training R2 -0.627971 | Validation loss 32.016544 | Validation R2 -1.503911
        Best loss 29.936550 | Best epoch 0001

100%|##########| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 7.3291, 10.1608, 10.0233,  9.8829], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.401255 | Training R2 -0.358544 | Validation loss 28.629280 | Validation R2 -1.002123
        Best loss 28.629280 | Best epoch 0004

100%|##########| 672/672 [01:28<00:00,  7.58it/s]
tensor([14.4474, 19.8099, 19.4276, 18.6136, 23.0821, 21.7736, 26.9981, 26.1418,
        24.3684, 28.5206, 26.5152], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836])

        Epoch 0005 | Training loss 19.169922 | Training R2 0.005122 | Validation loss 21.290998 | Validation R2 -0.107291
        Best loss 21.290998 | Best epoch 0005

100%|##########| 672/672 [01:29<00:00,  7.49it/s]
tensor([12.2309, 18.9201, 18.0805, 16.3241, 20.7797, 18.8313, 22.8460, 20.6343,
        24.4485, 21.9717], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0006 | Training loss 19.678331 | Training R2 -0.048349 | Validation loss 22.492300 | Validation R2 -0.235770
        Best loss 21.290998 | Best epoch 0005

100%|##########| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 9.0321, 16.7148, 15.5704, 14.4203], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0007 | Training loss 18.438383 | Training R2 0.079604 | Validation loss 20.871935 | Validation R2 -0.064132
```

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        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################################################################################################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 0.2794,  0.7751,  0.5484, -0.3596, -1.0415, -1.9528, -2.6358, -3.3204,
        -2.3768, -4.0057, -5.6395], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0008 | Training loss 20.370321 | Training R2 -0.123375 | Validation loss 23.957869 | Validation R2 -0.402059
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################################################################################################################################################| 672/672 [01:31<00:00,  7.38it/s]
tensor([17.7417, 27.3907, 25.9303], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0009 | Training loss 19.084763 | Training R2 0.013942 | Validation loss 21.900980 | Validation R2 -0.171647
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################################################################################################################################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([17.3056, 25.6101, 24.2517, 20.7280, 26.5591, 24.9605, 21.8946, 26.8496,
        25.2540, 22.2393], grad_fn=<IndexBackward0>)
tensor([17.8830, 55.3190, 16.9870,  2.1271, 56.8470, 17.5230,  2.1942, 57.7130,
        17.7900,  2.2277])

        Epoch 0010 | Training loss 17.859404 | Training R2 0.136499 | Validation loss 20.114540 | Validation R2 0.011697
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################################################################################################################################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([ 8.7530, 19.8132, 16.8510, 16.2882, 22.7456, 19.5403, 19.2723],
       grad_fn=<IndexBackward0>)
tensor([ 9.2660, 25.5950,  5.0055,  3.7205, 26.2690,  4.4291,  3.8185])

        Epoch 0011 | Training loss 18.237335 | Training R2 0.099566 | Validation loss 20.373814 | Validation R2 -0.013945
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################################################################################################################################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 9.9975, 15.6876, 13.4450, 11.2903, 17.1275, 15.1765, 11.2384],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727])

        Epoch 0012 | Training loss 17.548340 | Training R2 0.166316 | Validation loss 19.443098 | Validation R2 0.076577
        Best loss 19.443098 | Best epoch 0012

100%|##########################################################################################################################################################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 9.9177, 18.4395, 17.9721, 17.5216, 14.3823, 12.5939, 11.2551,  9.9186,
        16.4753, 13.0444], grad_fn=<IndexBackward0>)
tensor([ 4.1835, 35.5470, 29.2780, 24.3620,  6.9018,  3.3599,  1.9581,  1.1412,
        14.7460,  4.1835])

        Epoch 0013 | Training loss 17.206947 | Training R2 0.198439 | Validation loss 19.141432 | Validation R2 0.105009
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################################################################################################################################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([12.4364, 27.2565, 23.2694, 19.6116, 16.4919, 29.9886, 27.1892, 23.8359,
        20.2024], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243])

        Epoch 0014 | Training loss 17.306837 | Training R2 0.189105 | Validation loss 19.362793 | Validation R2 0.084189
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################################################################################################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([ 9.0598, 20.0499, 19.4907, 18.9320, 17.8166, 16.1479, 12.2752, 10.0752,
         8.9788, 18.8787, 14.2877, 10.3545,  8.6562, 18.4221, 14.3182, 10.7028,
         9.1701], grad_fn=<IndexBackward0>)
tensor([ 1.7205, 44.0430, 33.8580, 27.3170, 18.5670, 10.6030,  2.8810,  1.3684,
         0.9431, 27.6900,  6.1533,  1.6721,  0.9567, 23.0690,  6.2359,  1.6946,
         0.9695])

        Epoch 0015 | Training loss 16.755896 | Training R2 0.239911 | Validation loss 19.031542 | Validation R2 0.115256
        Best loss 19.031542 | Best epoch 0015

100%|##########################################################################################################################################################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([  0.9582,   1.0904,   0.4565,  -1.8299,  -3.4424,  -5.5529,  -7.1404,
        -8.7248,  -7.3052, -10.9318, -14.4289], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0016 | Training loss 16.645119 | Training R2 0.249928 | Validation loss 18.393700 | Validation R2 0.173566
        Best loss 18.393700 | Best epoch 0016

100%|##########################################################################################################################################################################################################| 672/672 [01:40<00:00,  6.68it/s]
tensor([ 6.8242, 20.9803, 15.5757, 10.6441,  6.5071, 20.2602, 15.3891, 10.3295,
         6.6992, 19.2614, 16.2208, 12.1368,  8.1876], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581])

        Epoch 0017 | Training loss 16.093096 | Training R2 0.298854 | Validation loss 17.970434 | Validation R2 0.211163
        Best loss 17.970434 | Best epoch 0017

100%|##########################################################################################################################################################################################################| 672/672 [01:38<00:00,  6.79it/s]
tensor([12.8932, 35.1585, 29.2565, 17.6236, 35.2379, 31.1231, 21.2395],
       grad_fn=<IndexBackward0>)
tensor([ 3.8765, 62.3080, 16.2100,  1.3937, 63.5960, 16.5530,  1.4231])

        Epoch 0018 | Training loss 15.311383 | Training R2 0.365315 | Validation loss 16.984724 | Validation R2 0.295328
        Best loss 16.984724 | Best epoch 0018

100%|##########################################################################################################################################################################################################| 672/672 [01:47<00:00,  6.26it/s]
tensor([16.5482, 29.7475, 28.0376], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0019 | Training loss 14.230635 | Training R2 0.451751 | Validation loss 15.854136 | Validation R2 0.386019
        Best loss 15.854136 | Best epoch 0019

100%|##########################################################################################################################################################################################################| 672/672 [02:00<00:00,  5.57it/s]
tensor([19.7466, 42.1145, 30.2606, 14.1118, 37.6893, 25.5962, 11.4744, 34.7414,
        11.2551, 33.2510, 23.2312, 11.2077, 33.0895, 23.2144, 11.2046, 32.8959,
        23.1463, 11.2140, 32.9500, 23.3397, 11.3844, 32.9221, 23.4265, 11.5103,
        23.5826, 11.6663, 32.9310, 23.6521, 11.7840, 32.9144, 23.7639],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0020 | Training loss 12.025496 | Training R2 0.608497 | Validation loss 13.721763 | Validation R2 0.540072
        Best loss 13.721763 | Best epoch 0020

100%|##########################################################################################################################################################################################################| 672/672 [02:26<00:00,  4.60it/s]
tensor([11.1434, 49.1650, 25.8507, 12.7483], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0021 | Training loss 12.230107 | Training R2 0.595061 | Validation loss 13.446256 | Validation R2 0.558356
        Best loss 13.446256 | Best epoch 0021

100%|##########################################################################################################################################################################################################| 672/672 [02:42<00:00,  4.13it/s]
tensor([ 7.8498, 35.5636, 31.8140, 27.4297, 23.8189, 15.3497, 39.8910, 28.7233,
        18.5893, 41.4949, 30.8928, 19.8995, 41.8754, 38.6326, 20.1299, 38.6822,
        20.5340, 38.5935, 21.5521], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590])

        Epoch 0022 | Training loss 9.790716 | Training R2 0.740488 | Validation loss 12.751149 | Validation R2 0.602837
        Best loss 12.751149 | Best epoch 0022

100%|##########################################################################################################################################################################################################| 672/672 [02:35<00:00,  4.31it/s]
tensor([14.1666, 61.5551, 29.6613,  8.8076, 58.5753, 24.2845,  8.8832],
       grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781])

        Epoch 0023 | Training loss 8.497423 | Training R2 0.804519 | Validation loss 10.855521 | Validation R2 0.712147
        Best loss 10.855521 | Best epoch 0023

100%|##########################################################################################################################################################################################################| 672/672 [02:43<00:00,  4.10it/s]
tensor([15.8495, 61.9667, 28.1483, 10.4488], grad_fn=<IndexBackward0>)
tensor([18.4370, 63.6710, 21.1850,  2.2930])

        Epoch 0024 | Training loss 7.026572 | Training R2 0.866335 | Validation loss 7.219308 | Validation R2 0.872690
        Best loss 7.219308 | Best epoch 0024

100%|##########################################################################################################################################################################################################| 672/672 [03:00<00:00,  3.72it/s]
tensor([15.0177, 53.2453, 22.2480, 13.1297, 52.0899, 24.2600],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])

        Epoch 0025 | Training loss 22.096283 | Training R2 -0.321805 | Validation loss 31.622337 | Validation R2 -1.442631
        Best loss 7.219308 | Best epoch 0024

100%|##########################################################################################################################################################################################################| 672/672 [03:02<00:00,  3.69it/s]
tensor([ 9.0573, 64.8458, 19.9370,  7.2607,  4.3328, 59.8810, 18.9035,  3.8537],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0026 | Training loss 6.403774 | Training R2 0.888980 | Validation loss 6.044273 | Validation R2 0.910760
        Best loss 6.044273 | Best epoch 0026

100%|##########################################################################################################################################################################################################| 672/672 [02:55<00:00,  3.82it/s]
tensor([ 6.9223, 61.5160, 18.7082,  3.0362, 18.1905,  2.9401, 18.2441,  2.8033],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559])

        Epoch 0027 | Training loss 6.205529 | Training R2 0.895747 | Validation loss 6.115032 | Validation R2 0.908659
        Best loss 6.044273 | Best epoch 0026

100%|##########################################################################################################################################################################################################| 672/672 [02:55<00:00,  3.84it/s]
tensor([ 6.6950, 60.9784, 50.3774, 41.8519, 28.7659, 16.2084,  8.8678,  3.7320,
         2.6390], grad_fn=<IndexBackward0>)
```

```
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6446,
         4.3127])

        Epoch 0028 | Training loss 6.358976 | Training R2 0.890528 | Validation loss 5.888662 | Validation R2 0.915296
        Best loss 5.888662 | Best epoch 0028

100%|##########################################################################################################################################################################################################################################| 672/672 [02:53<00:00,  3.87it/s]
tensor([ 5.4355, 52.7556, 12.8180,  2.5391], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0029 | Training loss 6.320073 | Training R2 0.891863 | Validation loss 5.790334 | Validation R2 0.918101
        Best loss 5.790334 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 3 --model 4 --save fold_3 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################################################################################################################################################################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 2.8724,  6.5957,  6.8080,  6.9899,  7.2021, 10.7213, 10.9348, 11.3314,
        14.8272, 15.0422, 15.1036, 15.4413, 18.9374, 19.1537, 19.5554, 23.0516,
        23.2693, 23.6736, 27.3578, 27.6082, 27.7960, 30.7728, 30.9930, 31.2133],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666,
        61.4260, 21.6510, 16.6580,  3.9438, 61.4060, 21.6430,  3.9424, 61.4240,
        21.6460,  3.9429, 24.6850,  8.6517,  3.9430, 52.7130, 18.6040,  7.4356])

        Epoch 0001 | Training loss 25.439198 | Training R2 -0.752008 | Validation loss 31.925747 | Validation R2 -1.489729
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################################################################################################################################################################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([ 3.2931,  5.3593,  5.3786,  5.3980,  5.4173,  5.4752,  7.2988,  7.3569,
         7.4149,  9.1766,  9.2347,  9.2928, 11.0515, 11.1676, 12.9117, 13.0278,
        14.7861, 14.9023, 16.6606, 16.7768, 18.5066, 18.6228, 20.3668, 20.4830,
        22.2271, 22.3433, 24.1067, 24.2035, 25.9476, 26.0638, 27.7936, 27.9099,
        29.6397, 29.7559, 31.4857, 31.6020, 33.4481, 35.1973, 35.2942, 37.0240,
        37.1403, 38.8701, 38.9864, 40.7162, 40.8325, 42.5338, 42.6501, 44.3800,
        44.4963, 46.1862, 46.2250], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0002 | Training loss 26.376934 | Training R2 -0.883553 | Validation loss 34.834122 | Validation R2 -1.964010
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################################################################################################################################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([ 7.8250, 11.8784, 11.8799, 11.8814, 11.8873, 11.8917, 11.8975, 11.9019,
        11.9062, 15.7652, 15.7763, 15.7875], grad_fn=<IndexBackward0>)
tensor([ 2.8854, 42.8980, 34.5060, 27.9840, 12.2340,  6.5823,  2.8806,  1.5499,
         0.8339, 54.9410, 12.2540,  2.8854])

        Epoch 0003 | Training loss 24.805820 | Training R2 -0.665852 | Validation loss 32.632885 | Validation R2 -1.601243
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################################################################################################################################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 8.7386, 11.7069, 11.5418, 11.3754, 11.2797, 11.2316, 13.9237, 13.7604,
        13.6669, 13.6202, 16.3320, 16.2147, 16.1207, 16.0738],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8804,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0004 | Training loss 22.594074 | Training R2 -0.382033 | Validation loss 29.154833 | Validation R2 -1.076304
        Best loss 29.154833 | Best epoch 0004

100%|##########################################################################################################################################################################################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([13.8576, 17.9291, 17.4015, 16.8603], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0005 | Training loss 19.321512 | Training R2 -0.010675 | Validation loss 21.662233 | Validation R2 -0.146242
        Best loss 21.662233 | Best epoch 0005

100%|##########################################################################################################################################################################################################################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([11.5918, 16.2894, 16.0552], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0006 | Training loss 18.806362 | Training R2 0.042500 | Validation loss 20.810762 | Validation R2 -0.057903
        Best loss 20.810762 | Best epoch 0006

100%|##########################################################################################################################################################################################################################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([13.7967, 24.9147, 23.5840, 22.4126, 21.0541, 27.8658, 26.2462, 23.2119],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0007 | Training loss 18.502975 | Training R2 0.073144 | Validation loss 20.257120 | Validation R2 -0.002364
        Best loss 20.257120 | Best epoch 0007

100%|##########################################################################################################################################################################################################################################| 672/672 [01:33<00:00,  7.18it/s]
tensor([ 7.3947, 16.2876, 14.5021], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0008 | Training loss 17.884424 | Training R2 0.134077 | Validation loss 19.712755 | Validation R2 0.050785
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################################################################################################################################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 7.4039, 16.9333, 14.2522], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0009 | Training loss 18.018396 | Training R2 0.121056 | Validation loss 20.877218 | Validation R2 -0.064670
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################################################################################################################################################################################| 672/672 [01:32<00:00,  7.24it/s]
tensor([0.6249, 7.8101, 7.3241, 3.8194, 1.0698], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0010 | Training loss 17.464170 | Training R2 0.174295 | Validation loss 20.522924 | Validation R2 -0.028841
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################################################################################################################################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 9.3226, 15.8665,  8.5315, 13.2728,  7.9733], grad_fn=<IndexBackward0>)
tensor([15.8300, 13.0430,  1.2608, 15.9120,  1.2850])

        Epoch 0011 | Training loss 15.910845 | Training R2 0.314645 | Validation loss 18.198824 | Validation R2 0.190985
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################################################################################################################################################################################| 672/672 [01:31<00:00,  7.38it/s]
tensor([ 4.3449, 16.5067], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0012 | Training loss 15.860810 | Training R2 0.318949 | Validation loss 18.750023 | Validation R2 0.141237
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################################################################################################################################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 8.7084, 25.3828, 17.3558,  9.8191,  3.7226,  1.3463, 10.4619,  6.1137,
         2.9816, 10.1290,  7.5545,  4.8109,  4.4536], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0013 | Training loss 13.904661 | Training R2 0.476580 | Validation loss 15.886896 | Validation R2 0.383479
        Best loss 15.886896 | Best epoch 0013

100%|##########################################################################################################################################################################################################################################| 672/672 [01:35<00:00,  7.05it/s]
tensor([ 7.0433, 27.5600, 16.8307,  7.2308,  0.1864,  9.9691,  3.3722, -0.6687,
         7.9856,  3.2674, -0.1207], grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866,
        16.0580,  5.2932,  1.7451])

        Epoch 0014 | Training loss 12.929752 | Training R2 0.547405 | Validation loss 15.179044 | Validation R2 0.437194
        Best loss 15.179044 | Best epoch 0014

100%|##########################################################################################################################################################################################################################################| 672/672 [01:33<00:00,  7.15it/s]
tensor([ 7.4332, 30.5729, 16.2396], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0015 | Training loss 12.248608 | Training R2 0.593835 | Validation loss 14.446182 | Validation R2 0.490228
        Best loss 14.446182 | Best epoch 0015

100%|##########################################################################################################################################################################################################################################| 672/672 [01:35<00:00,  7.01it/s]
tensor([ 4.6836,  7.6980,  7.1804, 17.4322, 10.2643,  9.2834, 19.8746, 11.5507,
        10.7448, 13.1053, 12.3932, 20.9605, 14.0527, 22.7131, 18.8298],
       grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462,  3.2262,  2.3463, 25.6730,  2.3549, 30.2890,  8.4665])

        Epoch 0016 | Training loss 11.735577 | Training R2 0.627147 | Validation loss 14.173969 | Validation R2 0.509258
        Best loss 14.173969 | Best epoch 0016

100%|##########################################################################################################################################################################################################################################| 672/672 [01:37<00:00,  6.89it/s]
tensor([11.6500, 60.2137, 25.1021, 10.0511], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])
```

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        Epoch 0017 | Training loss 10.962422 | Training R2 0.674656 | Validation loss 14.000322 | Validation R2 0.521209
        Best loss 14.000322 | Best epoch 0017

100%|########################################################################################################################| 672/672 [01:42<00:00,  6.55it/s]
tensor([ 1.9511, 20.6897,  3.2896, -2.9803, -5.5958, 20.0863,  5.9632, -0.5994,
        -4.8749, 19.8183,  6.0784, -1.1292, -4.3055, 19.2795,  7.1646,  0.7781,
        -3.7093], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900, 35.4880,  5.5170,  0.8985,  0.1896, 35.4880,  7.1499,  1.5090,
         0.1896])

        Epoch 0018 | Training loss 8.945731 | Training R2 0.783349 | Validation loss 10.094747 | Validation R2 0.751079
        Best loss 10.094747 | Best epoch 0018

100%|########################################################################################################################| 672/672 [02:03<00:00,  5.46it/s]
tensor([18.3829, 63.2539, 23.4179,  4.5281, 46.1589, 19.9410,  4.2955, 35.4959,
        16.3430,  3.1342, 26.7132, 12.0767,  3.3039,  2.6298],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775])

        Epoch 0019 | Training loss 8.820597 | Training R2 0.789368 | Validation loss 9.154214 | Validation R2 0.795303
        Best loss 9.154214 | Best epoch 0019

100%|########################################################################################################################| 672/672 [02:19<00:00,  4.81it/s]
tensor([ 4.1644, 14.0128, -0.3138, 27.2210, 10.2752, -0.3314, 23.0703,  7.9699,
        -0.3345], grad_fn=<IndexBackward0>)
tensor([ 1.7265, 18.3160,  2.4943, 49.3870, 15.7180,  2.1405, 40.9940, 12.9500,
         1.7635])

        Epoch 0020 | Training loss 7.317793 | Training R2 0.855026 | Validation loss 7.885971 | Validation R2 0.848092
        Best loss 7.885971 | Best epoch 0020

100%|########################################################################################################################| 672/672 [02:29<00:00,  4.49it/s]
tensor([ 8.4705, 47.7004, 13.9731,  1.0199, 41.2189, 11.3355,  1.4946, 40.8871,
        13.6375,  2.4164, 39.6342, 12.4571,  3.1625], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0021 | Training loss 7.042254 | Training R2 0.865738 | Validation loss 8.384834 | Validation R2 0.828265
        Best loss 7.885971 | Best epoch 0020

100%|########################################################################################################################| 672/672 [02:34<00:00,  4.36it/s]
tensor([ 4.4215, 36.0008,  8.1078,  0.6668, -1.3523, -1.4276, 11.2206, -0.1053,
        -1.8685, -1.9566,  9.4959, -0.7273, -2.5235, -2.5964,  8.4442, -2.1228,
        -3.3086, -3.3706], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307])

        Epoch 0022 | Training loss 9.585545 | Training R2 0.751250 | Validation loss 10.479862 | Validation R2 0.731724
        Best loss 7.885971 | Best epoch 0020

100%|########################################################################################################################| 672/672 [02:33<00:00,  4.38it/s]
tensor([ 7.7273, 48.1425, 12.7922,  1.4126, 44.4121, 10.8110,  1.8589, 44.7639,
        13.0078,  1.6967, 44.0305, 10.4389,  1.3453], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0023 | Training loss 6.300526 | Training R2 0.892531 | Validation loss 5.878633 | Validation R2 0.915584
        Best loss 5.878633 | Best epoch 0023
```


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 68%|########################################################################################################################7                                          | 68%|####################################
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tensor([ 4.2463, 36.7811,  8.6615,  1.4889, -0.0500, -0.0957, 12.9539,  1.7627,
         0.3970,  0.3455, 12.1383,  1.8436,  0.3857,  0.3445, 11.9547,  1.1080,
         0.2285,  0.1806, 11.7720,  1.7816,  0.1001,  7.4648,  1.6911,  0.0825,
        11.4667,  0.7494, -0.1261, -0.1730,  0.2474, -0.3031, 30.3681,  6.5845,
         0.4806, -0.2833], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.8910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307, 10.7730,  2.1190,  0.3304,  6.7693,  2.1190,  0.3304,
        10.7810,  1.6811,  0.4171,  0.3307,  1.0556,  0.3304, 35.8960,  6.7693,
         1.3316,  0.4168])

        Epoch 0024 | Training loss 6.111111 | Training R2 0.898896 | Validation loss 5.680680 | Validation R2 0.921174
        Best loss 5.680680 | Best epoch 0024

100%|##############| 672/672 [02:42<00:00,  4.14it/s]
tensor([ 8.8150, 11.5567,  4.6076, 11.2782,  5.0257,  6.5838,  5.3709, 11.5210,
         5.6812, 11.6247,  5.9075, 11.7576,  6.1699, 12.0414,  6.4387, 12.2436],
       grad_fn=<IndexBackward0>)
tensor([14.5460, 14.3260,  2.1336, 15.1440,  2.2555,  7.1526,  2.2158, 14.6630,
         2.1838, 14.4490,  2.1519, 14.3450,  2.1365, 14.4340,  2.1497, 14.5460])

        Epoch 0025 | Training loss 6.472453 | Training R2 0.886586 | Validation loss 7.626081 | Validation R2 0.857940
        Best loss 5.680680 | Best epoch 0024

100%|##############| 672/672 [02:50<00:00,  3.95it/s]
tensor([ 1.5432,  6.2264,  4.7843,  3.4637,  1.7148,  0.1873, -0.2482, -0.3312,
        -0.3259], grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0026 | Training loss 6.822579 | Training R2 0.873984 | Validation loss 8.459892 | Validation R2 0.825177
        Best loss 5.680680 | Best epoch 0024

100%|##############| 672/672 [02:51<00:00,  3.91it/s]
tensor([12.3268, 41.0046, 31.4636], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0027 | Training loss 6.095839 | Training R2 0.899400 | Validation loss 6.896765 | Validation R2 0.883812
        Best loss 5.680680 | Best epoch 0024

100%|##############| 672/672 [02:48<00:00,  3.98it/s]
tensor([ 3.3598, 38.0550, 32.1865, 26.7041, 11.2778,  5.3198,  1.1977, -0.6329,
        44.5308, 10.9635,  1.2176], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0028 | Training loss 6.544991 | Training R2 0.884030 | Validation loss 6.196602 | Validation R2 0.906206
        Best loss 5.680680 | Best epoch 0024

100%|##############| 672/672 [02:46<00:00,  4.04it/s]
tensor([ 5.3302, 57.8313, 14.6693,  3.2426,  1.1091, 15.5492,  4.6520,  2.3154,
        58.9284, 16.3087,  2.9490,  2.4515, 56.6236, 16.2949,  5.9694,  2.6612,
        20.1659,  6.1725,  3.0380, 20.9118,  6.8515,  3.4699],
       grad_fn=<IndexBackward0>)
tensor([ 0.8310, 59.4470, 12.7970,  2.9511,  0.8392, 12.6360,  2.9139,  0.8286,
        58.9270, 12.7180,  1.5640,  0.8341, 56.6760, 12.2320,  3.4784,  0.8022,
        15.3490,  3.5396,  0.8163, 15.6260,  3.6034,  0.8310])

        Epoch 0029 | Training loss 6.115059 | Training R2 0.898765 | Validation loss 7.040408 | Validation R2 0.878922
        Best loss 5.680680 | Best epoch 0024

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 3 --model 5 --save fold_3 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##############| 672/672 [01:37<00:00,  6.86it/s]
tensor([ 2.0993,  4.3603,  4.5242,  4.8280,  6.9204,  7.1301,  7.3631,  9.4930,
         9.6565,  9.9135, 12.0199, 12.2073, 12.4649], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0798,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225, 40.6640, 12.7280,  2.7241])

        Epoch 0001 | Training loss 24.240671 | Training R2 -0.590810 | Validation loss 29.148003 | Validation R2 -1.075331
        Best loss 29.148003 | Best epoch 0001

100%|##############| 672/672 [01:30<00:00,  7.44it/s]
tensor([4.3878, 7.2371, 7.3457], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0002 | Training loss 25.267263 | Training R2 -0.728405 | Validation loss 32.724815 | Validation R2 -1.615919
        Best loss 29.148003 | Best epoch 0001

100%|##############| 672/672 [01:30<00:00,  7.44it/s]
tensor([ 5.5793,  8.6449,  8.6271,  8.6107,  8.5985, 11.4784, 11.4660, 11.4518],
       grad_fn=<IndexBackward0>)
tensor([ 1.4091, 45.1660,  6.8944,  1.3910,  0.4434, 45.6640,  8.7781,  1.4091])

        Epoch 0003 | Training loss 24.392866 | Training R2 -0.610849 | Validation loss 31.869343 | Validation R2 -1.480939
        Best loss 29.148003 | Best epoch 0001

100%|##############| 672/672 [01:30<00:00,  7.43it/s]
tensor([ 5.8613, 10.4141, 10.1605,  9.9754], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0004 | Training loss 20.007446 | Training R2 -0.083708 | Validation loss 23.670774 | Validation R2 -0.368658
        Best loss 23.670774 | Best epoch 0004

100%|##############| 672/672 [01:29<00:00,  7.52it/s]
tensor([10.7725, 17.4414, 16.9693, 15.8382, 21.2687, 19.7636, 24.7900, 23.0800,
        27.9219, 25.9787], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0005 | Training loss 19.205898 | Training R2 0.001384 | Validation loss 22.241131 | Validation R2 -0.208325
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:29<00:00,  7.49it/s]
tensor([13.6329, 20.3223, 19.5666, 17.8168, 23.6848, 22.6136, 20.6065, 26.5026,
        25.2495, 23.9893, 22.9034], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])

        Epoch 0006 | Training loss 20.557449 | Training R2 -0.144109 | Validation loss 24.015671 | Validation R2 -0.408832
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:29<00:00,  7.54it/s]
tensor([16.9284, 21.8471, 20.9418, 20.8352, 20.7271, 20.3929, 23.8760, 23.4270,
        22.9282, 26.1789, 25.6684, 25.1570, 28.0688, 27.3257, 30.1612, 29.3570,
        32.1722, 31.3065, 34.1266, 33.1985, 35.9462, 34.9561, 37.6573, 36.6051,
        39.2385, 38.1246, 40.6862, 39.5110, 42.0308, 40.7943],
       grad_fn=<IndexBackward0>)
tensor([38.1730, 32.4920, 24.8420, 20.1090, 16.9610, 11.5390, 42.3870, 24.3350,
        16.9860, 47.3100, 27.9650, 19.6630, 34.2530, 20.9790, 35.0450, 21.5240,
        35.5990, 21.8790, 36.1540, 22.2220, 36.2560, 22.3030, 36.3190, 22.3450,
        36.2250, 22.2940, 36.0400, 22.1840, 35.9840, 22.1450])

        Epoch 0007 | Training loss 20.864714 | Training R2 -0.178566 | Validation loss 24.533953 | Validation R2 -0.470297
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:29<00:00,  7.54it/s]
tensor([13.5987, 17.2932, 17.1564, 17.0169], grad_fn=<IndexBackward0>)
tensor([31.1600, 21.5030, 17.4770, 14.5830])

        Epoch 0008 | Training loss 20.585428 | Training R2 -0.147226 | Validation loss 24.066521 | Validation R2 -0.414805
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 9.4386, 16.3450, 14.2150, 11.4437, 16.6023, 15.0743],
       grad_fn=<IndexBackward0>)
```

```
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0009 | Training loss 19.902319 | Training R2 -0.072350 | Validation loss 23.161474 | Validation R2 -0.310395
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:29<00:00,  7.54it/s]
tensor([ 5.5932, 12.3538, 12.0206, 11.6848, 10.3945,  9.4810,  8.2765,  7.3738],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0010 | Training loss 19.259192 | Training R2 -0.004165 | Validation loss 22.403614 | Validation R2 -0.226044
        Best loss 22.241131 | Best epoch 0005

100%|##############| 672/672 [01:30<00:00,  7.41it/s]
tensor([ 7.3921, 15.4699, 12.9607, 10.8167,  8.3234, 16.6326, 13.7868, 10.9830,
         8.6877, 16.5475, 14.0182, 11.2736,  8.7886, 15.5458, 13.3381, 10.9156,
         8.5450, 13.5284, 12.2548,  9.8752,  7.6965, 12.9978, 10.7930,  8.5555,
         6.4607, 11.1752,  9.0147,  5.6914,  4.6343,  6.9687,  4.7241,  2.6200,
         7.4725,  0.9743,  5.9411,  3.7118, -0.5238,  1.9366,  0.0317, -2.3644,
        -0.0617, -2.3752, -4.5300, -0.0170, -2.3218, -4.7410, -7.4294],
       grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866, 20.7580,  9.6001,  2.4950,  0.7861, 39.1950,  9.6000,  2.4949,
         0.7861, 37.7600,  9.2488,  1.3492,  0.7573,  9.2427,  2.4021,  0.7568,
        42.0710,  0.8422, 45.0040, 11.0200,  0.9023, 11.0300,  3.4749,  0.9031,
        11.0300,  2.8665,  0.9031, 45.0330, 11.0300,  2.8665,  0.7450])

        Epoch 0011 | Training loss 18.370600 | Training R2 0.086359 | Validation loss 20.881422 | Validation R2 -0.065099
        Best loss 20.881422 | Best epoch 0011

100%|##############| 672/672 [01:34<00:00,  7.14it/s]
tensor([ 6.5970, 11.4671,  7.1559, 11.7921,  9.5270,  7.0336, 11.2793,  9.2502,
         6.8160, 10.6249,  8.9877,  6.4109, 10.4517,  8.3311,  5.9003,  9.3980,
         5.0892,  8.5680,  6.4435,  3.8118,  7.4316,  5.2236,  2.4744,  6.0502,
         4.0339,  2.3123,  0.8804,  4.4167,  2.0192, -0.9629,  0.0474, -3.0528,
        -1.1970, -3.4589], grad_fn=<IndexBackward0>)
tensor([ 7.5182, 15.6800,  3.1867, 27.9940, 10.3060,  3.4217, 32.5420, 11.7100,
         3.4396, 32.5520, 13.2420,  3.4408, 40.3530, 12.2300,  3.5924, 29.4830,
         3.6040, 32.6680, 11.7570,  3.4535, 34.0010, 12.2340,  3.5934, 34.0970,
        13.8700,  6.6497,  3.6041, 34.1050, 12.2730,  3.6049, 12.2740,  3.6054,
        17.7370,  7.5182])

        Epoch 0012 | Training loss 17.796364 | Training R2 0.142584 | Validation loss 20.198370 | Validation R2 0.003442
        Best loss 20.198370 | Best epoch 0012

100%|##############| 672/672 [01:34<00:00,  7.10it/s]
tensor([18.1552, 22.1167, 18.2234, 23.1250, 20.6723, 16.5251, 21.2824, 18.8539,
        15.4051, 19.8181, 17.8533, 15.0033, 19.0660, 17.3397, 14.4262, 18.4159],
       grad_fn=<IndexBackward0>)
tensor([46.6430, 16.5660,  2.9642, 47.5600, 16.8100,  3.0078, 47.1240, 16.6500,
         2.9791, 47.5720, 16.8140,  3.0085, 47.0390, 16.6260,  2.9749, 46.6430])

        Epoch 0013 | Training loss 17.672243 | Training R2 0.154502 | Validation loss 20.135670 | Validation R2 0.009620
        Best loss 20.135670 | Best epoch 0013

100%|##############| 672/672 [01:32<00:00,  7.26it/s]
tensor([15.7235, 21.9340, 21.4483, 20.9525, 19.3949, 21.5689, 25.2046, 23.9585,
        22.7006, 25.1933, 23.5008, 25.3662, 24.0588, 26.2581, 24.4513, 26.5796,
        24.7060, 27.2621, 24.8573, 26.8676, 25.2804], grad_fn=<IndexBackward0>)
tensor([20.9330, 26.7620, 22.9870, 19.9020, 13.0070, 17.6410, 46.8390, 29.5720,
        19.3340, 35.8980, 20.3400, 31.7000, 20.7250, 36.8060, 20.8550, 36.8910,
        20.9040, 42.8090, 20.9210, 36.9340, 20.9280])

        Epoch 0014 | Training loss 16.964031 | Training R2 0.220911 | Validation loss 19.311337 | Validation R2 0.089050
        Best loss 19.311337 | Best epoch 0014

100%|##############| 672/672 [01:33<00:00,  7.18it/s]
tensor([17.8863, 37.3666, 32.3489, 23.9999, 39.5029, 35.9349, 28.6494, 38.7055,
        35.1126, 28.4681, 37.0100, 33.2479, 29.0802, 30.2658, 36.5677, 31.0483,
        37.3955, 35.5460, 32.0257, 38.4204, 36.4113, 32.7683],
       grad_fn=<IndexBackward0>)
tensor([ 6.5237, 74.1680, 27.8270,  6.0609, 78.2140, 29.7730,  6.4850, 78.5910,
        29.9390,  6.5212, 78.6230, 29.9530,  6.5243,  6.5245, 63.0610,  6.4075,
        64.1270, 29.9090,  6.5146, 78.6170, 29.9510,  6.5237])

        Epoch 0015 | Training loss 16.071217 | Training R2 0.300759 | Validation loss 18.356150 | Validation R2 0.176937
        Best loss 18.356150 | Best epoch 0015

100%|##############| 672/672 [01:34<00:00,  7.09it/s]
tensor([16.5277, 44.4044, 39.2769, 27.7244, 45.6794, 40.7189, 32.3551, 44.8518,
        38.4719, 30.6690], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.0520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.8935])

        Epoch 0016 | Training loss 16.231964 | Training R2 0.286701 | Validation loss 18.394156 | Validation R2 0.173525
        Best loss 18.356150 | Best epoch 0015

100%|##############| 672/672 [01:33<00:00,  7.16it/s]
tensor([ 5.3319, 17.4150, 16.5360, 15.6327, 11.7102,  8.7342,  5.1355,  2.4899],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0017 | Training loss 16.121244 | Training R2 0.296399 | Validation loss 18.390121 | Validation R2 0.173888
        Best loss 18.356150 | Best epoch 0015

100%|##############| 672/672 [01:32<00:00,  7.29it/s]
tensor([ 8.2026, 28.0302, 26.6790, 23.8754, 20.0850, 16.5093, 11.9295,  8.6301,
         5.4420, 24.6861, 16.0989,  8.5960,  4.5533, 18.9753, 15.0632,  9.7732,
         6.4840], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089])

        Epoch 0018 | Training loss 13.867579 | Training R2 0.479369 | Validation loss 15.791674 | Validation R2 0.390847
        Best loss 15.791674 | Best epoch 0018

100%|##############| 672/672 [01:38<00:00,  6.82it/s]
tensor([ 6.1014e+00,  2.5528e+01,  1.4262e+01,  5.9708e+00, -2.2717e+00,
         1.6885e+01, -6.1398e+00,  3.2727e-01, -3.4941e+00,  1.1665e+01,
         5.4953e+00,  3.5982e-01, -3.4189e+00,  1.1026e+01,  5.0514e+00,
         7.2515e-04, -3.6842e+00], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866])

        Epoch 0019 | Training loss 12.710710 | Training R2 0.562610 | Validation loss 14.843241 | Validation R2 0.461820
        Best loss 14.843241 | Best epoch 0019

100%|##########################################################################| 672/672 [01:46<00:00,  6.31it/s]
tensor([10.6566, 46.4687, 26.5691, 10.1913,  2.7001, 35.4857, 14.4463,  7.3089,
         1.1632], grad_fn=<IndexBackward0>)
tensor([ 4.6511, 55.9800, 16.9540,  4.6838,  2.0962, 47.9720, 12.9760,  5.8075,
         2.2130])

        Epoch 0020 | Training loss 11.812094 | Training R2 0.622269 | Validation loss 13.195599 | Validation R2 0.574668
        Best loss 13.195599 | Best epoch 0020

100%|##########################################################################| 672/672 [02:00<00:00,  5.56it/s]
tensor([10.1553, 18.2987,  5.9339,  0.7742, 24.4130, 11.2959,  0.2882, 10.9734,
         0.3400, 22.0324,  9.4522,  4.2867,  0.6211, 23.1974,  5.1732,  1.2618,
         0.8361,  8.2529,  1.1520, 23.7739,  4.9145,  1.9538,  1.5326,  9.5868],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727, 17.5920,
         2.8681, 53.1470,  2.9466,  6.7516,  2.9232, 53.6570,  7.9009,  3.4208,
         2.9753, 11.9150,  2.9524, 53.4760,  6.8475,  3.4086,  2.9648, 14.9510])

        Epoch 0021 | Training loss 10.502948 | Training R2 0.701358 | Validation loss 11.709469 | Validation R2 0.665077
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:24<00:00,  4.66it/s]
tensor([ 4.8642, 17.7674,  3.7490, -0.9090], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0022 | Training loss 9.577409 | Training R2 0.751672 | Validation loss 12.240973 | Validation R2 0.633983
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:41<00:00,  4.17it/s]
tensor([10.1105, 54.1474, 47.1999, 40.6521, 34.9629, 18.5855, 10.9887,  5.3792,
         3.3805], grad_fn=<IndexBackward0>)
tensor([12.0510, 55.0980, 40.4280, 31.6660, 25.7020, 12.4280,  7.3585,  3.6646,
         2.1727])

        Epoch 0023 | Training loss 7.726895 | Training R2 0.838364 | Validation loss 9.112268 | Validation R2 0.797174
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:36<00:00,  4.28it/s]
tensor([ 6.9046, 41.2925, 34.5210, 23.4426, 12.2643,  5.9188,  1.2359, -0.0414,
        -0.5284, 38.4061,  9.3305, -0.1065, -1.4874, 31.3701,  6.5284, -1.4669,
        -2.4291, 13.1051, -1.7246, -3.2997], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089, 18.7290,  4.4247,  1.6964])

        Epoch 0024 | Training loss 9.422968 | Training R2 0.759617 | Validation loss 9.542447 | Validation R2 0.777572
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:51<00:00,  3.92it/s]
tensor([23.6239, 67.3576, 30.3424, 17.5867, 53.2716, 29.3855, 18.8101, 57.4894,
        31.0669, 19.9989, 59.8965], grad_fn=<IndexBackward0>)
tensor([42.1750, 56.1960,  7.7854,  0.4302, 32.9930,  7.7374,  0.4275, 41.1230,
         7.5177,  0.4154, 42.1750])

        Epoch 0025 | Training loss 7.962917 | Training R2 0.828338 | Validation loss 9.609860 | Validation R2 0.774418
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [03:05<00:00,  3.63it/s]
tensor([  4.8900,  45.6167,   9.5987,   0.1051,  -0.9369,  39.9992,   8.5798,
         -0.3131,  -1.5515,  39.4073,   9.3195,  -0.3392,  -2.4984,  37.1201,
```

```
          8.8991,  -0.9208,  -3.5922,  35.8086,   8.4388,  -1.9218,  -4.8642,
         33.2721,   7.2729,  -3.1486,  -6.2217,  31.8621,   6.4087,  -4.3224,
         -7.6073,  29.6215,   4.9850,  -5.7174,  -8.7939,  28.9204,   4.0174,
         -6.7392,  -9.6808,   7.2845,  -6.6397, -10.4594,  26.3385,   1.3159,
         -8.2648, -11.1160,  24.3990,  -0.4381,  -9.1098, -11.8479,  21.2692,
         -2.0180,  -9.9808, -12.4354,  18.3305,  -3.3384, -13.0876,  -4.3371,
        -11.5662, -13.8299,  17.7920, -14.3870,  -4.9450, -12.6202, -15.1504],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2640,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0026 | Training loss 8.169349 | Training R2 0.819323 | Validation loss 8.430163 | Validation R2 0.826403
        Best loss 8.430163 | Best epoch 0026

100%|##########################################################################| 672/672 [03:02<00:00,  3.69it/s]
tensor([ 6.5499, 48.5983, 15.1371,  3.5329], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0027 | Training loss 6.878480 | Training R2 0.871910 | Validation loss 7.949504 | Validation R2 0.845635
        Best loss 7.949504 | Best epoch 0027

100%|##########################################################################| 672/672 [02:58<00:00,  3.76it/s]
tensor([22.4853, 65.2880, 29.7628, 19.7173, 17.9791, 57.3877, 28.7129, 17.0198,
        16.9415, 26.9971, 16.9828, 63.2698, 30.2553, 16.8464, 63.8235, 30.3975,
        16.6662, 63.3403], grad_fn=<IndexBackward0>)
tensor([54.4230, 51.9620, 17.0410,  7.0369,  2.5077, 43.8090, 17.6270,  3.0059,
         2.5940, 15.3480,  2.6174, 55.5800, 18.3240,  2.6966, 55.2450, 18.2160,
         2.6806, 54.4230])

        Epoch 0028 | Training loss 6.115299 | Training R2 0.898757 | Validation loss 5.728622 | Validation R2 0.919838
        Best loss 5.728622 | Best epoch 0028

100%|##########################################################################| 672/672 [02:56<00:00,  3.81it/s]
tensor([ 9.6481, 86.3610, 29.5480,  5.6376, 78.3233, 26.1667,  6.2007, 78.0224,
        24.1587,  6.6242], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.8520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.0935])

        Epoch 0029 | Training loss 6.373678 | Training R2 0.890021 | Validation loss 7.142794 | Validation R2 0.875375
        Best loss 5.728622 | Best epoch 0028

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 4 --model 1 --save fold_4 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:31<00:00,  7.36it/s]
tensor([ 2.8156,  6.4742,  6.6527,  6.8312,  6.9842, 10.4804, 10.6588],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0001 | Training loss 25.589478 | Training R2 -0.772768 | Validation loss 32.346756 | Validation R2 -1.555826
        Best loss 32.346756 | Best epoch 0001

100%|##########################################################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([1.9038, 5.0573, 5.0673, 5.1375, 5.1977], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0002 | Training loss 25.551172 | Training R2 -0.767465 | Validation loss 33.349823 | Validation R2 -1.716795
        Best loss 32.346756 | Best epoch 0001

100%|##########################################################################| 672/672 [01:35<00:00,  7.06it/s]
tensor([ 5.6753,  9.1968,  9.1520,  9.1070,  9.0680, 12.3688, 12.3259, 12.2829,
        12.2460, 15.6801, 15.6373, 15.5945, 15.5579, 18.8876, 18.8448, 18.8021,
        18.7654, 22.0656, 22.0229, 21.9801, 21.9435, 25.1256, 25.0829, 25.0402,
        25.0036, 28.1739, 28.1312, 28.0886, 28.0520, 31.1455, 31.1029, 31.0603,
        31.0238, 34.1763, 34.1337, 34.0912, 34.0547, 37.1030, 37.0544, 37.0118,
        40.1939, 40.1514, 40.1089, 40.0725, 43.2250, 43.1825, 43.1401, 43.1036,
        46.1381, 46.0957, 46.0532, 46.0168, 48.9333, 48.8989, 48.8121, 51.7009,
        51.6585, 51.6222, 54.7601, 54.6392, 57.7422, 57.6999, 57.6637],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2640,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0003 | Training loss 25.064499 | Training R2 -0.700776 | Validation loss 33.287090 | Validation R2 -1.706584
        Best loss 32.346756 | Best epoch 0001

100%|##########################################################################| 672/672 [01:38<00:00,  6.82it/s]
tensor([11.9925, 16.1087, 15.6565, 14.7926, 18.7813, 18.1950, 17.1649],
       grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517])

        Epoch 0004 | Training loss 19.580549 | Training R2 -0.037956 | Validation loss 22.115347 | Validation R2 -0.194696
        Best loss 22.115347 | Best epoch 0004

100%|##########################################################################| 672/672 [01:35<00:00,  7.03it/s]
tensor([11.7457, 16.1828, 15.2492], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0005 | Training loss 17.637089 | Training R2 0.157863 | Validation loss 18.753033 | Validation R2 0.140961
        Best loss 18.753033 | Best epoch 0005

100%|##########################################################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([18.9408, 25.6120, 24.2652, 21.7064, 27.7522, 26.0064, 22.9544, 28.8805,
        26.7267, 22.9661], grad_fn=<IndexBackward0>)
tensor([13.8520, 73.2560, 25.4040,  4.4909, 62.0640, 23.5240,  4.7517, 62.2630,
        23.6030,  4.7676])

        Epoch 0006 | Training loss 17.212334 | Training R2 0.197937 | Validation loss 18.404135 | Validation R2 0.172628
        Best loss 18.404135 | Best epoch 0006

100%|##########################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([ 7.4809, 16.4973, 14.5521, 12.8453, 11.8989, 10.8038, 14.5344, 11.6942,
         9.5260,  9.1614], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530])

        Epoch 0007 | Training loss 18.241096 | Training R2 0.099195 | Validation loss 21.649376 | Validation R2 -0.144882
        Best loss 18.404135 | Best epoch 0006

100%|##########################################################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([21.2631, 37.7968, 34.6989, 28.8175, 35.9441, 28.1752, 40.1245, 34.2910,
        23.3075, 27.6585, 19.4856, 23.0779, 19.0806, 24.1141, 21.9171],
       grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836, 23.7820,  3.2723, 61.1610, 20.1800])

        Epoch 0008 | Training loss 15.880821 | Training R2 0.317229 | Validation loss 17.267464 | Validation R2 0.271672
        Best loss 17.267464 | Best epoch 0008

100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([29.5514, 33.9478, 33.5019, 33.0550, 31.7080, 36.2872, 34.6281, 32.9590,
        35.4917, 33.4942, 37.8410, 33.2047, 37.4423, 32.1499, 36.2251, 30.2793,
        34.2453, 27.6422, 31.5599, 24.2538, 28.0946, 21.8433, 24.2154],
       grad_fn=<IndexBackward0>)
tensor([66.9750, 34.8300, 30.4850, 27.1220, 19.3810, 59.4210, 39.4690, 28.2220,
        45.4640, 32.5130, 71.1690, 34.2430, 72.7160, 35.0360, 72.9860, 35.1970,
        73.1260, 35.2700, 73.7120, 35.5420, 73.9550, 35.6660, 66.9750])

        Epoch 0009 | Training loss 15.588125 | Training R2 0.342165 | Validation loss 17.531309 | Validation R2 0.249244
        Best loss 17.267464 | Best epoch 0008

100%|##########################################################################| 672/672 [10:16<00:00,  1.09it/s]
tensor([22.3988, 44.0035, 38.3123, 27.5719, 42.2598, 33.7127, 17.9093, 31.7069,
        21.5951, 15.1084, 21.6086, 18.1968, 14.7075, 19.6320, 17.6338, 14.6714,
        18.9939, 17.1625, 14.7096, 18.3896, 16.8863, 14.2772, 17.6625, 16.0937,
        14.1760, 16.9282, 15.6259, 13.6606, 16.4278, 15.1709],
       grad_fn=<IndexBackward0>)
tensor([22.8850, 73.4140, 23.4880,  3.5482, 76.4500, 24.6180,  3.7189, 76.3100,
        24.5840,  3.7138, 76.0510, 21.1850,  3.7013, 75.8210, 24.4220,  3.6893,
        74.9130, 24.1510,  3.6483, 73.3630, 23.6320,  3.5700, 72.1350, 23.2310,
         3.5094, 70.4750, 19.6300,  3.4295, 70.9820, 22.8850])

        Epoch 0010 | Training loss 15.053199 | Training R2 0.386539 | Validation loss 16.905653 | Validation R2 0.301874
        Best loss 16.905653 | Best epoch 0010

  8%|#####8                                                         | 51/672 [00:06<01:04,  9.63it/s]  8%|######1                                                        | 54/672 [00:06<01:20,  7.70it/s]  8%|######3
                                                  | 55/672 [00:06<01:21,  7.56it/s]100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([18.1234, 47.1816, 39.9245], grad_fn=<IndexBackward0>)
tensor([ 7.2340, 79.9040, 30.3950])

        Epoch 0011 | Training loss 14.768456 | Training R2 0.409528 | Validation loss 16.615559 | Validation R2 0.325627
```

```
        Best loss 16.615559 | Best epoch 0011

100%|##########################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([11.6720, 32.8382, 24.0419,  7.9924, 23.3818, 12.4458,  8.1120, 14.4407,
         11.5844,  8.4578], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0790,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225])

        Epoch 0012 | Training loss 14.076530 | Training R2 0.463561 | Validation loss 15.982780 | Validation R2 0.376014
        Best loss 15.982780 | Best epoch 0012

100%|##########################################################################| 672/672 [01:33<00:00,  7.20it/s]
tensor([15.4169, 37.7438, 26.4691,  7.0804, 27.0034, 15.1891],
       grad_fn=<IndexBackward0>)
tensor([15.6310, 53.5120, 15.1840,  1.6724, 54.8710, 15.6310])

        Epoch 0013 | Training loss 13.712152 | Training R2 0.490973 | Validation loss 15.644684 | Validation R2 0.402134
        Best loss 15.644684 | Best epoch 0013

100%|##########################################################################| 672/672 [01:32<00:00,  7.29it/s]
tensor([12.0577, 36.3803, 23.6637, 11.4284,  3.9892, 24.7131, 13.2179,  7.2145,
         3.9259, 17.6060, 11.4485,  7.1599,  4.1087, 14.8795, 10.1405,  7.4436,
         5.7456, 12.6350, 10.5755,  8.8864,  7.3162, 13.0429, 11.6113,  9.6312,
         8.1763, 13.7002, 12.1540, 10.3492,  8.4799, 14.0624, 12.3707],
       grad_fn=<IndexBackward0>)
tensor([15.8670, 48.0290, 15.0320,  5.2611,  2.1393, 49.5140, 15.6140,  5.4648,
         2.2222, 49.5850, 15.6390,  5.4735,  2.2257, 49.6100, 15.6440,  5.4753,
         2.2264, 49.5890, 15.6410,  5.4740,  2.2259, 49.5930, 15.6410,  4.7118,
         2.2260, 49.5930, 15.6410,  5.4742,  2.2260, 50.3130, 15.8670])

        Epoch 0014 | Training loss 13.242213 | Training R2 0.525266 | Validation loss 15.322500 | Validation R2 0.426506
        Best loss 15.322500 | Best epoch 0014

100%|##########################################################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 5.4798, 30.7803, 14.7806,  2.5093, -1.7086,  8.5024,  1.9989, -1.6791],
       grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866])

        Epoch 0015 | Training loss 12.924088 | Training R2 0.547802 | Validation loss 14.716954 | Validation R2 0.470939
        Best loss 14.716954 | Best epoch 0015

100%|##########################################################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([15.6168, 55.2221, 16.2939,  8.2661, 24.2689], grad_fn=<IndexBackward0>)
tensor([16.1690, 59.8340,  5.3050,  1.4892, 16.1690])

        Epoch 0016 | Training loss 11.898344 | Training R2 0.616732 | Validation loss 14.322660 | Validation R2 0.498908
        Best loss 14.322660 | Best epoch 0016

100%|##########################################################################| 672/672 [01:31<00:00,  7.30it/s]
tensor([12.7216, 59.7177, 25.1669,  4.2772, 34.5799, 21.0603,  9.3780,  3.6991,
        31.5247, 18.5450,  8.8795,  3.1359, 25.5747, 15.5161,  5.9220],
       grad_fn=<IndexBackward0>)
tensor([ 4.0299, 69.1500, 18.3480,  1.7573, 53.2860, 17.7690,  5.0245,  1.7018,
        65.7810, 20.9510,  4.9462,  1.6753, 64.1100, 17.0690,  4.0299])

        Epoch 0017 | Training loss 11.401729 | Training R2 0.648058 | Validation loss 13.213898 | Validation R2 0.573487
        Best loss 13.213898 | Best epoch 0017

100%|##########################################################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([ 2.9063, 32.5171, 27.8092, 23.1816, 13.6546,  9.5199,  5.4563,  2.9917,
         0.8526, 27.3170, 15.6950,  7.0380,  3.1720, 24.6298, 14.8523,  8.5628,
         4.3510, 22.1035, 15.0576,  8.9973,  5.4540, 22.2026, 13.7354,  9.1169,
         6.3164, 22.1408, 14.2489,  9.6895,  7.1869, 21.7399, 14.4235, 10.2883,
         8.0124, 21.3545, 11.1481,  8.8666, 20.7642, 15.1376, 11.6578,  9.4312,
        20.2414, 15.3670, 12.0332, 10.2129, 21.1668, 16.4321, 13.0078, 10.8106,
        21.6568, 17.0286, 13.6380, 11.4462, 22.2054, 17.6234, 14.2651, 12.1728,
        18.4076, 15.0337], grad_fn=<IndexBackward0>)
tensor([ 2.7419, 28.6490, 21.3580, 16.8180,  8.8564,  4.9078,  2.5526,  1.5643,
         0.9587, 44.6470,  8.7898,  2.7858,  1.0463, 43.9280,  8.6592,  2.7445,
         1.0308, 44.7080,  8.8094,  2.7920,  1.0487, 45.3180,  7.5611,  2.8303,
         1.0630, 45.7270,  9.0111,  2.8560,  1.0727, 45.7350,  9.0137,  2.8568,
         1.0730, 46.3300,  2.8935,  1.0868, 44.3590,  8.7473,  2.7724,  1.0413,
        31.3930,  7.5594,  2.4035,  1.0628, 43.9420,  8.6636,  2.7459,  1.0313,
        43.7170,  8.6165,  2.7309,  1.0257, 43.3150,  8.5378,  2.7060,  1.0163,
         8.6510,  2.7419])

        Epoch 0018 | Training loss 10.813417 | Training R2 0.683441 | Validation loss 13.203379 | Validation R2 0.574166
        Best loss 13.203379 | Best epoch 0018

100%|##########################################################################| 672/672 [01:36<00:00,  6.99it/s]
tensor([ 9.7498, 40.5504, 13.2881,  0.8898, 25.9407, 14.4120,  2.2655,  1.0768,
        24.7947, 14.0786,  1.6502], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568])

        Epoch 0019 | Training loss 10.473630 | Training R2 0.703023 | Validation loss 13.268398 | Validation R2 0.569962
        Best loss 13.203379 | Best epoch 0018

100%|##########################################################################| 672/672 [01:37<00:00,  6.91it/s]
tensor([ 2.5559, 19.4985,  2.8311, 33.7559, 17.7553,  2.5439],
       grad_fn=<IndexBackward0>)
tensor([ 0.9887, 13.2440,  1.0495, 44.2920, 11.1530,  1.0742])

        Epoch 0020 | Training loss 9.496670 | Training R2 0.755842 | Validation loss 10.343183 | Validation R2 0.738677
        Best loss 10.343183 | Best epoch 0020

100%|##########################################################################| 672/672 [01:41<00:00,  6.61it/s]
tensor([ 6.5408, 27.2245, 21.7968, 17.0160, 14.4693,  9.4895, 26.6533, 19.8093,
        14.0566, 29.3762, 22.2869, 16.0390, 30.4389, 16.7182, 30.6311, 16.9595,
        30.6151, 17.0785, 30.7607, 17.0520, 30.7647, 16.8004, 30.8296, 16.6525,
        30.7940, 16.4834, 27.5907, 16.3012, 30.4290, 16.1035, 30.0555, 15.9718,
        29.7875, 15.9149, 29.5319, 15.9032, 15.8856, 26.1478, 15.8869, 28.9241,
        15.8869, 28.7300, 15.8838, 28.5423, 15.8782, 28.2471, 15.7892, 28.3878,
        15.8788, 28.1359, 23.1418], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0021 | Training loss 7.951676 | Training R2 0.828823 | Validation loss 8.662682 | Validation R2 0.816695
        Best loss 8.662682 | Best epoch 0021

100%|##########################################################################| 672/672 [01:46<00:00,  6.28it/s]
tensor([ 5.0714, 41.2239, 10.6933,  1.8153, -1.6648, 32.1178, 11.6598,  2.8483],
       grad_fn=<IndexBackward0>)
tensor([ 2.2708, 40.9040,  9.4533,  2.2722,  0.6695, 40.8030,  9.4476,  2.2708])

        Epoch 0022 | Training loss 7.609004 | Training R2 0.843258 | Validation loss 8.749406 | Validation R2 0.813006
        Best loss 8.662682 | Best epoch 0021

100%|##########################################################################| 672/672 [02:06<00:00,  5.32it/s]
tensor([ 7.4991, 41.7259, 10.5250,  2.0759, -0.8212, -0.1132],
       grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724])

        Epoch 0023 | Training loss 6.876002 | Training R2 0.872003 | Validation loss 6.808918 | Validation R2 0.886753
        Best loss 6.808918 | Best epoch 0023

100%|##########################################################################| 672/672 [02:27<00:00,  4.57it/s]
tensor([10.0532, 11.7258,  3.9000, 25.9815, 11.5955,  4.2005, 24.3615, 10.3238,
         4.2509], grad_fn=<IndexBackward0>)
tensor([16.2540, 16.8150,  3.7307, 46.7120, 18.2510,  4.0494, 39.1610, 16.6890,
         4.1575])

        Epoch 0024 | Training loss 6.344456 | Training R2 0.891027 | Validation loss 6.287634 | Validation R2 0.903429
        Best loss 6.287634 | Best epoch 0024

100%|##########################################################################| 672/672 [02:32<00:00,  4.41it/s]
tensor([ 1.6894, 23.4610,  3.5930, -1.5898, -2.5777, 30.9283,  8.1172,  1.3945,
        -1.0457], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900])

        Epoch 0025 | Training loss 7.193916 | Training R2 0.859893 | Validation loss 8.765650 | Validation R2 0.812311
        Best loss 6.287634 | Best epoch 0024

100%|##########################################################################| 672/672 [02:33<00:00,  4.37it/s]
tensor([ 8.8472, 41.0249,  8.3407,  2.1899, 36.6626, 12.1595],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0026 | Training loss 6.314091 | Training R2 0.892068 | Validation loss 7.142266 | Validation R2 0.875393
        Best loss 6.287634 | Best epoch 0024

100%|##########################################################################| 672/672 [02:38<00:00,  4.24it/s]
tensor([ 8.5633, 52.2498,  1.5635, 17.5187,  1.9039, 16.5124,  1.4483],
       grad_fn=<IndexBackward0>)
tensor([ 5.0480, 57.3470,  1.4345, 18.1510,  1.4741, 17.6580,  1.4340])

        Epoch 0027 | Training loss 6.055744 | Training R2 0.900719 | Validation loss 5.718658 | Validation R2 0.920116
        Best loss 5.718658 | Best epoch 0027

100%|##########################################################################| 672/672 [02:39<00:00,  4.20it/s]
tensor([ 7.0780, 42.2500, 11.1324,  3.1023,  1.2874,  2.6817, 21.2856,  6.6037,
         3.4198], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166])

        Epoch 0028 | Training loss 6.592818 | Training R2 0.882328 | Validation loss 7.770147 | Validation R2 0.852522
        Best loss 5.718658 | Best epoch 0027

100%|##########################################################################| 672/672 [02:38<00:00,  4.23it/s]
tensor([ 3.7971, 35.3375,  8.4819,  1.6825, -0.3244, -0.4051, 13.2231,  2.0788,
         0.1861,  0.0965, 12.3860,  2.4895,  0.1087,  0.0419],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
```

```
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0029 | Training loss 5.998502 | Training R2 0.902587 | Validation loss 5.604497 | Validation R2 0.923274
        Best loss 5.604497 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 4 --model 2 --save fold_4 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([2.1999, 5.6524, 5.8418, 6.1936, 9.4868, 9.8432],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521])

        Epoch 0001 | Training loss 24.587435 | Training R2 -0.636649 | Validation loss 29.936550 | Validation R2 -1.189140
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 4.9043,  8.9507,  9.0836,  9.2166,  9.3305, 13.3845, 13.5179, 13.6512,
        13.7654, 17.8186, 17.9522, 18.0858], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243, 63.0070, 16.7890,  4.7756])

        Epoch 0002 | Training loss 25.483650 | Training R2 -0.758136 | Validation loss 33.067993 | Validation R2 -1.671072
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.59it/s]
tensor([ 7.6014, 11.0011, 11.0285], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0003 | Training loss 24.522160 | Training R2 -0.627971 | Validation loss 32.016544 | Validation R2 -1.503911
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 7.3291, 10.1608, 10.0233,  9.8829], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.401255 | Training R2 -0.358544 | Validation loss 28.629280 | Validation R2 -1.002123
        Best loss 28.629280 | Best epoch 0004

100%|##########################################################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([14.4474, 19.8099, 19.4276, 18.6136, 23.0821, 21.7736, 26.9981, 26.1418,
        24.3684, 28.5206, 26.5152], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836])

        Epoch 0005 | Training loss 19.169922 | Training R2 0.005122 | Validation loss 21.290998 | Validation R2 -0.107291
        Best loss 21.290998 | Best epoch 0005

100%|##########################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([12.2309, 18.9201, 18.0805, 16.3241, 20.7797, 18.8313, 22.8460, 20.6343,
        24.4485, 21.9717], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0006 | Training loss 19.678331 | Training R2 -0.048349 | Validation loss 22.492300 | Validation R2 -0.235770
        Best loss 21.290998 | Best epoch 0005

100%|##########################################################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([ 9.0321, 16.7148, 15.5704, 14.4203], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0007 | Training loss 18.438383 | Training R2 0.079604 | Validation loss 20.871935 | Validation R2 -0.064132
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:32<00:00,  7.23it/s]
tensor([ 0.2794,  0.7751,  0.5484, -0.3596, -1.0415, -1.9520, -2.6358, -3.3204,
        -2.3768, -4.0857, -5.6395], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0008 | Training loss 20.370321 | Training R2 -0.123375 | Validation loss 23.957869 | Validation R2 -0.402059
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([17.7417, 27.3907, 25.9303], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0009 | Training loss 19.084763 | Training R2 0.013942 | Validation loss 21.900980 | Validation R2 -0.171647
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([17.3056, 25.6101, 24.2517, 20.7280, 26.5591, 24.9605, 21.8946, 26.8496,
        25.2540, 22.2393], grad_fn=<IndexBackward0>)
tensor([17.8830, 55.3190, 16.9870,  2.1271, 56.8470, 17.5230,  2.1942, 57.7130,
        17.7900,  2.2277])

        Epoch 0010 | Training loss 17.859404 | Training R2 0.136499 | Validation loss 20.114540 | Validation R2 0.011697
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([ 8.7530, 19.8132, 16.8510, 16.2882, 22.7456, 19.5403, 19.2723],
       grad_fn=<IndexBackward0>)
tensor([ 9.2660, 25.5950,  5.0055,  3.7205, 26.2690,  4.4291,  3.8185])

        Epoch 0011 | Training loss 18.237335 | Training R2 0.099566 | Validation loss 20.373814 | Validation R2 -0.013945
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([ 9.9975, 15.6876, 13.4450, 11.2903, 17.1275, 15.1765, 11.2384],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727])

        Epoch 0012 | Training loss 17.548340 | Training R2 0.166316 | Validation loss 19.443098 | Validation R2 0.076577
        Best loss 19.443098 | Best epoch 0012

100%|##########################################################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([ 9.9177, 18.4395, 17.9721, 17.5216, 14.3823, 12.5939, 11.2551,  9.9186,
        16.4753, 13.0444], grad_fn=<IndexBackward0>)
tensor([ 4.1835, 35.5470, 29.2780, 24.3620,  6.9018,  3.3599,  1.9581,  1.1412,
        14.7460,  4.1835])

        Epoch 0013 | Training loss 17.206947 | Training R2 0.198439 | Validation loss 19.141432 | Validation R2 0.105009
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([12.4364, 27.2565, 23.2694, 19.6116, 16.4919, 29.9886, 27.1892, 23.8359,
        20.2024], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243])

        Epoch 0014 | Training loss 17.306837 | Training R2 0.189105 | Validation loss 19.362793 | Validation R2 0.084189
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([ 9.0598, 20.0499, 19.4907, 18.9320, 17.8166, 16.1479, 12.2752, 10.0752,
         8.9788, 18.8787, 14.2877, 10.3545,  8.6562, 18.4221, 14.3182, 10.7028,
         9.1701], grad_fn=<IndexBackward0>)
tensor([ 1.7205, 44.0430, 33.8580, 27.3170, 18.5670, 10.6030,  2.8810,  1.3684,
         0.9431, 27.6900,  6.1533,  1.6721,  0.9567, 23.0690,  6.2359,  1.6946,
         0.9695])

        Epoch 0015 | Training loss 16.755896 | Training R2 0.239911 | Validation loss 19.031542 | Validation R2 0.115256
        Best loss 19.031542 | Best epoch 0015

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([  0.9582,   1.0904,   0.4565,  -1.8299,  -3.4424,  -5.5529,  -7.1404,
         -8.7248,  -7.3052, -10.9318, -14.4289], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0016 | Training loss 16.645119 | Training R2 0.249928 | Validation loss 18.393700 | Validation R2 0.173566
        Best loss 18.393700 | Best epoch 0016

100%|##########################################################################| 672/672 [01:34<00:00,  7.12it/s]
tensor([ 6.8242, 20.9803, 15.5757, 10.6441,  6.5071, 20.2602, 15.3891, 10.3295,
         6.6992, 19.2614, 16.2280, 12.1368,  8.1876], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581])

        Epoch 0017 | Training loss 16.093096 | Training R2 0.298854 | Validation loss 17.970434 | Validation R2 0.211163
        Best loss 17.970434 | Best epoch 0017

100%|##########################################################################| 672/672 [01:40<00:00,  6.68it/s]
tensor([12.8932, 35.1585, 29.2565, 17.6236, 35.2379, 31.1231, 21.2395],
       grad_fn=<IndexBackward0>)
tensor([ 3.8765, 62.3080, 16.2100,  1.3937, 63.5960, 16.5530,  1.4231])

        Epoch 0018 | Training loss 15.311383 | Training R2 0.365315 | Validation loss 16.984724 | Validation R2 0.295328
        Best loss 16.984724 | Best epoch 0018

100%|##########################################################################| 672/672 [01:50<00:00,  6.07it/s]
tensor([16.5482, 29.7475, 28.0376], grad_fn=<IndexBackward0>)
```

```
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0019 | Training loss 14.230635 | Training R2 0.451751 | Validation loss 15.854136 | Validation R2 0.386019
        Best loss 15.854136 | Best epoch 0019

100%|##################################################################################| 672/672 [02:03<00:00,  5.43it/s]
tensor([19.7466, 42.1145, 30.2606, 14.1118, 37.6893, 25.5962, 11.4744, 34.7414,
        11.2551, 33.2510, 23.2312, 11.2077, 33.0895, 23.2144, 11.2046, 32.8959,
        23.1463, 11.2140, 32.9500, 23.3397, 11.3844, 32.9221, 23.4265, 11.5103,
        23.5826, 11.6663, 32.9310, 23.6521, 11.7840, 32.9144, 23.7639],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0020 | Training loss 12.025496 | Training R2 0.608497 | Validation loss 13.721763 | Validation R2 0.540072
        Best loss 13.721763 | Best epoch 0020

100%|##################################################################################| 672/672 [02:26<00:00,  4.59it/s]
tensor([11.1434, 49.1650, 25.8507, 12.7483], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0021 | Training loss 12.230107 | Training R2 0.595061 | Validation loss 13.446256 | Validation R2 0.558356
        Best loss 13.446256 | Best epoch 0021

100%|##################################################################################| 672/672 [02:45<00:00,  4.07it/s]
tensor([ 7.8498, 35.5636, 31.8140, 27.4297, 23.8189, 15.3497, 39.8910, 28.7233,
        18.5893, 41.4949, 30.8928, 19.8995, 41.8754, 38.6326, 20.1299, 38.6822,
        20.5340, 38.5935, 21.5521], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.8460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590])

        Epoch 0022 | Training loss 9.790716 | Training R2 0.740488 | Validation loss 12.751149 | Validation R2 0.602837
        Best loss 12.751149 | Best epoch 0022

100%|##################################################################################| 672/672 [02:44<00:00,  4.09it/s]
tensor([14.1666, 61.5551, 29.6613,  8.8076, 58.5753, 24.2845,  8.8832],
       grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781])

        Epoch 0023 | Training loss 8.497423 | Training R2 0.804519 | Validation loss 10.855521 | Validation R2 0.712147
        Best loss 10.855521 | Best epoch 0023

100%|##################################################################################| 672/672 [02:50<00:00,  3.94it/s]
tensor([15.8495, 61.9667, 28.1483, 10.4488], grad_fn=<IndexBackward0>)
tensor([18.4370, 63.6710, 21.1850,  2.2930])

        Epoch 0024 | Training loss 7.026572 | Training R2 0.866335 | Validation loss 7.219308 | Validation R2 0.872690
        Best loss 7.219308 | Best epoch 0024

100%|##################################################################################| 672/672 [03:09<00:00,  3.55it/s]
tensor([15.0177, 53.2453, 22.2480, 13.1297, 52.0899, 24.2600],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])

        Epoch 0025 | Training loss 22.096283 | Training R2 -0.321805 | Validation loss 31.622337 | Validation R2 -1.442631
        Best loss 7.219308 | Best epoch 0024

100%|##################################################################################| 672/672 [03:06<00:00,  3.60it/s]
tensor([ 9.0573, 64.0458, 19.9370,  7.2607,  4.3328, 59.8810, 18.9035,  3.8537],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0026 | Training loss 6.403774 | Training R2 0.888980 | Validation loss 6.044273 | Validation R2 0.910760
        Best loss 6.044273 | Best epoch 0026

100%|##################################################################################| 672/672 [03:06<00:00,  3.61it/s]
tensor([ 6.9223, 61.5160, 18.7082,  3.0362, 18.1905,  2.9401, 18.2441,  2.8033],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559])

        Epoch 0027 | Training loss 6.205529 | Training R2 0.895747 | Validation loss 6.115032 | Validation R2 0.908659
        Best loss 6.044273 | Best epoch 0026

100%|##################################################################################| 672/672 [03:05<00:00,  3.62it/s]
tensor([ 6.6950, 60.9784, 50.3774, 41.8519, 28.7659, 16.2084,  8.8678,  3.7320,
         2.6390], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0028 | Training loss 6.358976 | Training R2 0.890528 | Validation loss 5.888662 | Validation R2 0.915296
        Best loss 5.888662 | Best epoch 0028

100%|##################################################################################| 672/672 [03:03<00:00,  3.67it/s]
tensor([ 5.4355, 52.7556, 12.8180,  2.5391], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0029 | Training loss 6.320073 | Training R2 0.891863 | Validation loss 5.790334 | Validation R2 0.918101
        Best loss 5.790334 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 4 --model 3 --save fold_4 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##################################################################################| 672/672 [01:34<00:00,  7.08it/s]
tensor([ 2.8724,  6.5957,  6.8080,  6.9899,  7.2021, 10.7213, 10.9348, 11.3314,
        14.8272, 15.8422, 15.1036, 15.4413, 18.9374, 19.1537, 19.5554, 23.8516,
        23.2693, 23.6736, 27.3578, 27.6082, 27.7960, 30.7728, 30.9930, 31.2133],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666,
        61.4260, 21.6510, 16.6580,  3.9438, 61.4060, 21.6430,  3.9424, 61.4240,
        21.6460,  3.9429, 24.6850,  8.6517,  3.9430, 52.7130, 18.6040,  7.4356])

        Epoch 0001 | Training loss 25.439198 | Training R2 -0.752008 | Validation loss 31.925747 | Validation R2 -1.489729
        Best loss 31.925747 | Best epoch 0001

100%|##################################################################################| 672/672 [01:34<00:00,  7.11it/s]
tensor([ 3.2931,  5.3593,  5.3786,  5.3980,  5.4173,  5.4752,  7.2988,  7.3569,
         7.4149,  9.1766,  9.2347,  9.2928, 11.0515, 11.1676, 12.9117, 13.0278,
        14.7861, 14.9023, 16.6606, 16.7768, 18.5066, 18.6228, 20.3668, 20.4830,
        22.2271, 22.3433, 24.1067, 24.2035, 25.9476, 26.0638, 27.7936, 27.9099,
        29.6397, 29.7559, 31.4857, 31.6020, 33.4481, 35.1973, 35.2942, 37.0240,
        37.1403, 38.8701, 38.9864, 40.7162, 40.8325, 42.5338, 42.6501, 44.3800,
        44.4963, 46.1862, 46.2250], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0002 | Training loss 26.376934 | Training R2 -0.883553 | Validation loss 34.834122 | Validation R2 -1.964010
        Best loss 31.925747 | Best epoch 0001

100%|##################################################################################| 672/672 [01:34<00:00,  7.14it/s]
tensor([ 7.8250, 11.8784, 11.8799, 11.8814, 11.8873, 11.8917, 11.8975, 11.9019,
        11.9062, 15.7652, 15.7763, 15.7875], grad_fn=<IndexBackward0>)
tensor([ 2.8854, 42.8980, 34.5060, 27.9840, 12.2340,  6.5823,  2.8806,  1.5499,
         0.8339, 54.9410, 12.2540,  2.8854])

        Epoch 0003 | Training loss 24.805820 | Training R2 -0.665852 | Validation loss 32.632885 | Validation R2 -1.601243
        Best loss 31.925747 | Best epoch 0001

100%|##################################################################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 8.7386, 11.7069, 11.5418, 11.3754, 11.2797, 11.2316, 13.9237, 13.7604,
        13.6669, 13.6202, 16.3320, 16.2147, 16.1207, 16.0738],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8004,
         3.8889,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0004 | Training loss 22.594074 | Training R2 -0.382033 | Validation loss 29.154833 | Validation R2 -1.076304
        Best loss 29.154833 | Best epoch 0004

100%|##################################################################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([13.8576, 17.9291, 17.4015, 16.8603], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0005 | Training loss 19.321512 | Training R2 -0.010675 | Validation loss 21.662233 | Validation R2 -0.146242
        Best loss 21.662233 | Best epoch 0005

100%|##################################################################################| 672/672 [01:35<00:00,  7.05it/s]
tensor([11.5918, 16.2894, 16.0552], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0006 | Training loss 18.806362 | Training R2 0.042500 | Validation loss 20.810762 | Validation R2 -0.057903
        Best loss 20.810762 | Best epoch 0006

100%|##################################################################################| 672/672 [01:35<00:00,  7.06it/s]
tensor([13.7967, 24.9167, 23.5840, 22.4126, 21.0541, 27.8658, 26.2462, 23.2119],
       grad_fn=<IndexBackward0>)
```

```
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0007 | Training loss 18.502975 | Training R2 0.073144 | Validation loss 20.257120 | Validation R2 -0.002364
        Best loss 20.257120 | Best epoch 0007

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 7.3947, 16.2876, 14.5021], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0008 | Training loss 17.884424 | Training R2 0.134077 | Validation loss 19.712755 | Validation R2 0.050785
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([ 7.4039, 16.9333, 14.2522], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0009 | Training loss 18.018396 | Training R2 0.121056 | Validation loss 20.877218 | Validation R2 -0.064670
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([0.6249, 7.8101, 7.3241, 3.8194, 1.8698], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0010 | Training loss 17.464170 | Training R2 0.174295 | Validation loss 20.522924 | Validation R2 -0.028841
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 9.3226, 15.8665,  8.5315, 13.2728,  7.9733], grad_fn=<IndexBackward0>)
tensor([15.8300, 13.0430,  1.2608, 15.9120,  1.2850])

        Epoch 0011 | Training loss 15.910845 | Training R2 0.314645 | Validation loss 18.198824 | Validation R2 0.190985
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([ 4.3449, 16.5067], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0012 | Training loss 15.860810 | Training R2 0.318949 | Validation loss 18.750023 | Validation R2 0.141237
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([ 8.7084, 25.3828, 17.3558,  9.8191,  3.7226,  1.3463, 10.4619,  6.1137,
         2.9816, 10.1290,  7.5545,  4.8109,  4.4536], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0013 | Training loss 13.904661 | Training R2 0.476580 | Validation loss 15.886896 | Validation R2 0.383479
        Best loss 15.886896 | Best epoch 0013

100%|##########################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 7.0433, 27.5600, 16.8307,  7.2308,  0.1864,  9.9691,  3.3722, -0.6687,
         7.9856,  3.2674, -0.1207], grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866,
        16.0580,  5.2932,  1.7451])

        Epoch 0014 | Training loss 12.929752 | Training R2 0.547405 | Validation loss 15.179044 | Validation R2 0.437194
        Best loss 15.179044 | Best epoch 0014

100%|##########################################################################| 672/672 [01:34<00:00,  7.08it/s]
tensor([ 7.4332, 30.5729, 16.2396], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0015 | Training loss 12.248608 | Training R2 0.593835 | Validation loss 14.446182 | Validation R2 0.490228
        Best loss 14.446182 | Best epoch 0015

100%|##########################################################################| 672/672 [01:34<00:00,  7.12it/s]
tensor([ 4.6836,  7.6980,  7.1804, 17.4322, 10.2643,  9.2034, 19.8746, 11.5507,
        10.7448, 13.1053, 12.3932, 20.9605, 14.8527, 22.7131, 18.8298],
       grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462,  3.2262,  2.3463, 25.6730,  2.3549, 30.2890,  8.4665])

        Epoch 0016 | Training loss 11.735577 | Training R2 0.627147 | Validation loss 14.173969 | Validation R2 0.509258
        Best loss 14.173969 | Best epoch 0016

100%|##########################################################################| 672/672 [01:37<00:00,  6.86it/s]
tensor([11.6500, 60.2137, 25.1021, 10.0511], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0017 | Training loss 10.962422 | Training R2 0.674656 | Validation loss 14.000322 | Validation R2 0.521209
        Best loss 14.000322 | Best epoch 0017

100%|##########################################################################| 672/672 [01:43<00:00,  6.51it/s]
tensor([ 1.9511, 20.6897,  3.2896, -2.9803, -5.5958, 20.0863,  5.9632, -0.5994,
        -4.8749, 19.8183,  6.0784, -1.1292, -4.3055, 19.2795,  7.1646,  0.7781,
        -3.7093], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900, 35.4880,  5.5170,  0.8985,  0.1896, 35.4880,  7.1499,  1.5090,
         0.1896])

        Epoch 0018 | Training loss 8.945731 | Training R2 0.783349 | Validation loss 10.094747 | Validation R2 0.751079
        Best loss 10.094747 | Best epoch 0018

100%|##########################################################################| 672/672 [02:06<00:00,  5.32it/s]
tensor([18.3829, 63.2539, 23.4179,  4.5281, 46.1589, 19.9410,  4.2955, 35.4959,
        16.3430,  3.1342, 26.7132, 12.0767,  3.3039,  2.6298],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775])

        Epoch 0019 | Training loss 8.820597 | Training R2 0.789368 | Validation loss 9.154214 | Validation R2 0.795303
        Best loss 9.154214 | Best epoch 0019

100%|##########################################################################| 672/672 [02:21<00:00,  4.75it/s]
tensor([ 4.1644, 14.0128, -0.3138, 27.2210, 10.2752, -0.3314, 23.0703,  7.9699,
        -0.3345], grad_fn=<IndexBackward0>)
tensor([ 1.7265, 18.3160,  2.4943, 49.3870, 15.7180,  2.1405, 40.9940, 12.9500,
         1.7635])

        Epoch 0020 | Training loss 7.317793 | Training R2 0.855026 | Validation loss 7.885971 | Validation R2 0.848092
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:26<00:00,  4.59it/s]
tensor([ 8.4705, 47.7004, 13.9731,  1.0199, 41.2189, 11.3355,  1.4946, 40.8871,
        13.6375,  2.4164, 39.6342, 12.4571,  3.1625], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0021 | Training loss 7.042254 | Training R2 0.865738 | Validation loss 8.384834 | Validation R2 0.828265
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:36<00:00,  4.29it/s]
tensor([ 4.4215, 36.0008,  8.1078,  0.6668, -1.3523, -1.4276, 11.2206, -0.1053,
        -1.8685, -1.9566,  9.4959, -0.7273, -2.5235, -2.5964,  8.4442, -2.1228,
        -3.3086, -3.3706], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307])

        Epoch 0022 | Training loss 9.585545 | Training R2 0.751250 | Validation loss 10.479862 | Validation R2 0.731724
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:37<00:00,  4.27it/s]
tensor([ 7.7273, 48.1425, 12.7922,  1.4126, 44.4121, 10.8110,  1.8589, 44.7639,
        13.0078,  1.6967, 44.0305, 10.4389,  1.3453], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0023 | Training loss 6.300526 | Training R2 0.892531 | Validation loss 5.878633 | Validation R2 0.915584
        Best loss 5.878633 | Best epoch 0023

100%|##########################################################################| 672/672 [02:38<00:00,  4.24it/s]
tensor([ 4.2463, 36.7811,  8.6615,  1.4889, -0.0500, -0.0957, 12.9539,  1.7627,
         0.3970,  0.3455, 12.1383,  1.8436,  0.3857,  0.3445, 11.9547,  1.1080,
         0.2285,  0.1806, 11.7720,  1.7816,  0.1001,  7.4648,  1.6911,  0.0825,
        11.4667,  0.7494, -0.1261, -0.1730,  0.2474, -0.3031, 30.3681,  6.5845,
         0.4806, -0.2833], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307, 10.7730,  2.1190,  0.3304,  6.7693,  2.1190,  0.3304,
        10.7810,  1.6811,  0.4171,  0.3307,  1.0556,  0.3304, 35.8960,  6.7693,
         1.3316,  0.4168])

        Epoch 0024 | Training loss 6.111111 | Training R2 0.898896 | Validation loss 5.680680 | Validation R2 0.921174
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:43<00:00,  4.12it/s]
tensor([ 8.8150, 11.5567,  4.6076, 11.2782,  5.0257,  6.5838,  5.3709, 11.5210,
         5.6812, 11.6247,  5.9075, 11.7576,  6.1699, 12.0414,  6.4387, 12.2436],
       grad_fn=<IndexBackward0>)
tensor([14.5460, 14.3260,  2.1336, 15.1440,  2.2555,  7.1526,  2.2158, 14.6630,
         2.1838, 14.4490,  2.1519, 14.3450,  2.1365, 14.4340,  2.1497, 14.5460])

        Epoch 0025 | Training loss 6.472453 | Training R2 0.886586 | Validation loss 7.626081 | Validation R2 0.857940
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:50<00:00,  3.95it/s]
tensor([ 1.5432,  6.2264,  4.7043,  3.4637,  1.7148,  0.1873, -0.2482, -0.3312,
        -0.3259], grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0026 | Training loss 6.822579 | Training R2 0.873984 | Validation loss 8.459892 | Validation R2 0.825177
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:51<00:00,  3.92it/s]
tensor([12.3268, 41.0046, 31.4636], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0027 | Training loss 6.095839 | Training R2 0.899400 | Validation loss 6.896765 | Validation R2 0.883812
```

```
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:48<00:00,  3.98it/s]
tensor([ 3.3598, 38.0550, 32.1865, 26.7041, 11.2778,  5.3198,  1.1977, -0.6329,
         44.5308, 10.9635,  1.2176], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0028 | Training loss 6.544991 | Training R2 0.884030 | Validation loss 6.196602 | Validation R2 0.906206
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:43<00:00,  4.10it/s]
tensor([ 5.3302, 57.8313, 14.6693,  3.2426,  1.1091, 15.5492,  4.6520,  2.3154,
        58.9204, 16.3087,  2.9490,  2.4515, 56.6236, 16.2949,  5.9694,  2.6612,
        20.1659,  6.1725,  3.0380, 20.9118,  6.8515,  3.4699],
       grad_fn=<IndexBackward0>)
tensor([ 0.8310, 59.4470, 12.7970,  2.9511,  0.8392, 12.6360,  2.9139,  0.8286,
        58.9270, 12.7180,  1.5640,  0.8341, 56.6760, 12.2320,  3.4784,  0.8022,
        15.3490,  3.5396,  0.8163, 15.6260,  3.6034,  0.8310])

        Epoch 0029 | Training loss 6.115059 | Training R2 0.898765 | Validation loss 7.040408 | Validation R2 0.878922
        Best loss 5.680680 | Best epoch 0024

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 4 --model 4 --save fold_4 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:33<00:00,  7.19it/s]
tensor([ 2.0993,  4.3603,  4.5242,  4.8280,  6.9204,  7.1301,  7.3631,  9.4930,
         9.6565,  9.9135, 12.0199, 12.2073, 12.4649], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0798,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225, 40.6640, 12.7280,  2.7241])

        Epoch 0001 | Training loss 24.240671 | Training R2 -0.590810 | Validation loss 29.148003 | Validation R2 -1.075331
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([4.3878, 7.2371, 7.3457], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0002 | Training loss 25.267263 | Training R2 -0.728405 | Validation loss 32.724815 | Validation R2 -1.615919
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([ 5.5793,  8.6449,  8.6271,  8.6107,  8.5985, 11.4784, 11.4660, 11.4518],
       grad_fn=<IndexBackward0>)
tensor([ 1.4091, 45.1660,  6.8944,  1.3910,  0.4434, 45.6640,  8.7781,  1.4091])

        Epoch 0003 | Training loss 24.392866 | Training R2 -0.610849 | Validation loss 31.869343 | Validation R2 -1.480939
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 5.8613, 10.4141, 10.1605,  9.9754], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0004 | Training loss 20.007446 | Training R2 -0.083708 | Validation loss 23.670774 | Validation R2 -0.368658
        Best loss 23.670774 | Best epoch 0004

100%|##########################################################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([10.7725, 17.4414, 16.9693, 15.8382, 21.2687, 19.7636, 24.7900, 23.0800,
         27.9219, 25.9787], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2860,  2.0559,
        15.0810,  2.0389])

        Epoch 0005 | Training loss 19.205898 | Training R2 0.001384 | Validation loss 22.241131 | Validation R2 -0.208325
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([13.6329, 20.3223, 19.5666, 17.8168, 23.6848, 22.6136, 20.6065, 26.5026,
        25.2495, 23.9893, 22.9034], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])

        Epoch 0006 | Training loss 20.557449 | Training R2 -0.144109 | Validation loss 24.015671 | Validation R2 -0.408832
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([16.9284, 21.8471, 20.9418, 20.8352, 20.7271, 20.3929, 23.8760, 23.4270,
         22.9282, 26.1789, 25.6684, 25.1570, 28.0688, 27.3257, 30.1612, 29.3570,
        32.1722, 31.3065, 34.1266, 33.1985, 35.9462, 34.9561, 37.6573, 36.6051,
        39.2385, 38.1246, 40.6862, 39.5110, 42.0308, 40.7943],
       grad_fn=<IndexBackward0>)
tensor([38.1730, 32.4920, 24.8420, 20.1090, 16.9610, 11.5390, 42.3870, 24.3350,
        16.9860, 47.3100, 27.9650, 19.6630, 34.2530, 20.9790, 35.0450, 21.5240,
        35.5990, 21.8790, 36.1540, 22.2220, 36.2560, 22.3030, 36.3190, 22.3450,
        36.2250, 22.2940, 36.0400, 22.1840, 35.9840, 22.1450])

        Epoch 0007 | Training loss 20.864714 | Training R2 -0.178566 | Validation loss 24.533953 | Validation R2 -0.470297
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([13.5987, 17.2932, 17.1564, 17.0169], grad_fn=<IndexBackward0>)
tensor([31.1600, 21.5030, 17.4770, 14.5830])

        Epoch 0008 | Training loss 20.585428 | Training R2 -0.147226 | Validation loss 24.066521 | Validation R2 -0.414805
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([ 9.4386, 16.3450, 14.2150, 11.4437, 16.6023, 15.0743],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0009 | Training loss 19.902319 | Training R2 -0.072350 | Validation loss 23.161474 | Validation R2 -0.310395
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:30<00:00,  7.42it/s]
tensor([ 5.5932, 12.3538, 12.0206, 11.6848, 10.3945,  9.4810,  8.2765,  7.3738],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0010 | Training loss 19.259192 | Training R2 -0.004165 | Validation loss 22.403614 | Validation R2 -0.226044
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 7.3921, 15.4699, 12.9607, 10.8167,  8.3234, 16.6326, 13.7868, 10.9830,
         8.6877, 16.5475, 14.0182, 11.2736,  8.7886, 15.5458, 13.3381, 10.9156,
         8.5450, 13.5284, 12.2548,  9.8752,  7.6965, 12.9978, 10.7930,  8.5555,
         6.4607, 11.1752,  9.0147,  5.6914,  4.6343,  6.9687,  4.7241,  2.6200,
         7.4725,  0.9743,  5.9411,  3.7118, -0.5238,  1.9366,  0.0317, -2.3644,
        -0.0617, -2.3752, -4.5300, -0.0170, -2.3218, -4.7410, -7.4294],
       grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866, 20.7580,  9.6001,  2.4950,  0.7861, 39.1950,  9.6000,  2.4949,
         0.7861, 37.7600,  9.2488,  1.3492,  0.7573,  9.2427,  2.4021,  0.7568,
        42.0710,  0.8422, 45.0040, 11.0200,  0.9023, 11.0300,  3.4749,  0.9831,
        11.0300,  2.8665,  0.9031, 45.0330, 11.0300,  2.8665,  0.7450])

        Epoch 0011 | Training loss 18.378600 | Training R2 0.086359 | Validation loss 20.881422 | Validation R2 -0.065099
        Best loss 20.881422 | Best epoch 0011

100%|##########################################################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([ 6.5970, 11.4671,  7.1559, 11.7921,  9.5270,  7.0336, 11.2793,  9.2502,
         6.8160, 10.6249,  8.9877,  6.4109, 10.4517,  8.3311,  5.9003,  9.3980,
         5.0892,  8.5680,  6.4435,  3.8118,  7.4316,  5.2236,  2.4744,  6.0502,
         4.0339,  2.3123,  0.8804,  4.4167,  2.0192, -0.9629,  0.0474, -3.0528,
        -1.1970, -3.4509], grad_fn=<IndexBackward0>)
tensor([ 7.5182, 15.6800,  3.1867, 27.9940, 10.3060,  3.4217, 32.5420, 11.7100,
         3.4396, 32.5520, 13.2420,  3.4408, 40.3530, 12.2300,  3.5924, 29.4830,
         3.6040, 32.6680, 11.7570,  3.4535, 34.0010, 12.2340,  3.5934, 34.0970,
        13.8700,  6.6497,  3.6041, 34.1050, 12.2730,  3.6049, 12.2740,  3.6054,
        17.7370,  7.5182])

        Epoch 0012 | Training loss 17.796364 | Training R2 0.142584 | Validation loss 20.198370 | Validation R2 0.003442
        Best loss 20.198370 | Best epoch 0012

100%|##########################################################################| 672/672 [01:29<00:00,  7.49it/s]
tensor([18.1552, 22.1167, 18.2234, 23.1250, 20.6723, 16.5251, 21.2824, 18.8539,
        15.4051, 19.8181, 17.8533, 15.0033, 19.0660, 17.3397, 14.4262, 18.4159],
       grad_fn=<IndexBackward0>)
tensor([46.6430, 16.5660,  2.9642, 47.5600, 16.8100,  3.0078, 47.1240, 16.6500,
         2.9791, 47.5720, 16.8140,  3.0085, 47.0390, 16.6260,  2.9749, 46.6430])

        Epoch 0013 | Training loss 17.672243 | Training R2 0.154502 | Validation loss 20.135670 | Validation R2 0.009620
        Best loss 20.135670 | Best epoch 0013

100%|##########################################################################| 672/672 [01:31<00:00,  7.36it/s]
tensor([15.7235, 21.9340, 21.4483, 20.9525, 19.3949, 21.5689, 25.2046, 23.9585,
        22.7006, 25.1933, 23.5008, 25.3662, 24.0588, 26.2581, 24.4513, 26.5796,
        24.7060, 27.2621, 24.8573, 26.8676, 25.2804], grad_fn=<IndexBackward0>)
tensor([20.9330, 26.7620, 22.9870, 19.9020, 13.0070, 17.6410, 46.8390, 29.5720,
        19.3340, 35.8980, 20.3400, 31.7000, 20.7250, 36.8060, 20.8550, 36.8910,
        20.9040, 42.8090, 20.9210, 36.9340, 20.9280])
```

```
        Epoch 0014 | Training loss 16.964031 | Training R2 0.220911 | Validation loss 19.311337 | Validation R2 0.089050
        Best loss 19.311337 | Best epoch 0014

100%|##########################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([17.8863, 37.3666, 32.3489, 23.9999, 39.5029, 35.9349, 28.6494, 38.7055,
        35.1126, 28.4681, 37.0100, 33.2479, 29.0802, 30.2658, 36.5677, 31.0483,
        37.3955, 35.5460, 32.0257, 38.4204, 36.4113, 32.7683],
       grad_fn=<IndexBackward0>)
tensor([ 6.5237, 74.1680, 27.8270,  6.0609, 78.2140, 29.7730,  6.4850, 78.5910,
        29.9390,  6.5212, 78.6230, 29.9530,  6.5243,  6.5245, 63.0610,  6.4075,
        64.1270, 29.9090,  6.5146, 78.6170, 29.9510,  6.5237])

        Epoch 0015 | Training loss 16.071217 | Training R2 0.300759 | Validation loss 18.356150 | Validation R2 0.176937
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([16.5277, 44.4044, 39.2769, 27.7244, 45.6794, 40.7189, 32.3551, 44.8518,
        38.4719, 30.6690], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.0520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.0935])

        Epoch 0016 | Training loss 16.231964 | Training R2 0.286701 | Validation loss 18.394156 | Validation R2 0.173525
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:31<00:00,  7.37it/s]
tensor([ 5.3319, 17.4150, 16.5360, 15.6327, 11.7102,  8.7342,  5.1355,  2.4899],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0017 | Training loss 16.121244 | Training R2 0.296399 | Validation loss 18.390121 | Validation R2 0.173888
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:32<00:00,  7.25it/s]
tensor([ 8.2026, 28.0302, 26.6790, 23.8754, 20.0850, 16.5093, 11.9295,  8.6301,
         5.4420, 24.6861, 16.0909,  8.5960,  4.5533, 18.9753, 15.0632,  9.7732,
         6.4840], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089])

        Epoch 0018 | Training loss 13.867579 | Training R2 0.479369 | Validation loss 15.791674 | Validation R2 0.390847
        Best loss 15.791674 | Best epoch 0018

100%|##########################################################################| 672/672 [01:38<00:00,  6.84it/s]
tensor([ 6.1014e+00,  2.5528e+01,  1.4262e+01,  5.9708e+00, -2.2717e+00,
         1.6885e+01,  6.1398e+00,  3.2727e-01, -3.4941e+00,  1.1665e+01,
         5.4953e+00,  3.5982e-01, -3.4189e+00,  1.1026e+01,  5.0514e+00,
         7.2515e-04, -3.6842e+00], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866])

        Epoch 0019 | Training loss 12.710710 | Training R2 0.562610 | Validation loss 14.843241 | Validation R2 0.461820
        Best loss 14.843241 | Best epoch 0019

100%|##########################################################################| 672/672 [01:46<00:00,  6.32it/s]
tensor([10.6566, 46.4687, 26.5691, 10.1913,  2.7001, 35.4857, 14.4463,  7.3089,
         1.1632], grad_fn=<IndexBackward0>)
tensor([ 4.6511, 55.9800, 16.9540,  4.6838,  2.0962, 47.9720, 12.9760,  5.8075,
         2.2130])

        Epoch 0020 | Training loss 11.812094 | Training R2 0.622269 | Validation loss 13.195599 | Validation R2 0.574668
        Best loss 13.195599 | Best epoch 0020

100%|##########################################################################| 672/672 [02:00<00:00,  5.60it/s]
tensor([10.1553, 18.2987,  5.9339,  0.7742, 24.4130, 11.2959,  0.2882, 10.9734,
         0.3400, 22.8324,  0.4522,  4.2867,  0.6211, 23.1974,  5.1732,  1.2618,
         0.8361,  8.2529,  1.1520, 23.7739,  4.9145,  1.9538,  1.5326,  9.5868],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727, 17.5920,
         2.8681, 53.1470,  2.9466,  6.7516,  2.9232, 53.6570,  7.9009,  3.4208,
         2.9753, 11.9150,  2.9524, 53.4760,  6.8475,  3.4086,  2.9648, 14.9510])

        Epoch 0021 | Training loss 10.502948 | Training R2 0.701358 | Validation loss 11.709469 | Validation R2 0.665077
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:23<00:00,  4.67it/s]
tensor([ 4.8642, 17.7674,  3.7490, -0.9098], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0022 | Training loss 9.577409 | Training R2 0.751672 | Validation loss 12.240973 | Validation R2 0.633983
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:37<00:00,  4.26it/s]
tensor([10.1105, 54.1474, 47.1999, 40.6521, 34.9629, 18.5855, 10.9887,  5.3792,
         3.3805], grad_fn=<IndexBackward0>)
tensor([12.0510, 55.0980, 40.4280, 31.6660, 25.7020, 12.4280,  7.3585,  3.6646,
         2.1727])

        Epoch 0023 | Training loss 7.726895 | Training R2 0.838364 | Validation loss 9.112268 | Validation R2 0.797174
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:34<00:00,  4.35it/s]
tensor([ 6.9046, 41.2925, 34.5210, 23.4426, 12.2643,  5.9188,  1.2359, -0.0414,
        -0.5284, 38.4061,  9.3305, -0.1065, -1.4874, 31.3701,  6.5284, -1.4669,
        -2.4291, 13.1051, -1.7246, -3.2997], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089, 18.7290,  4.4247,  1.6964])

        Epoch 0024 | Training loss 9.422968 | Training R2 0.759617 | Validation loss 9.542447 | Validation R2 0.777572
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:47<00:00,  4.02it/s]
tensor([23.6239, 67.3576, 30.3424, 17.5867, 53.2716, 29.3855, 18.8101, 57.4894,
        31.0669, 19.9989, 59.8965], grad_fn=<IndexBackward0>)
tensor([42.1750, 56.1960,  7.7854,  0.4302, 32.9930,  7.7374,  0.4275, 41.1230,
         7.5177,  0.4154, 42.1750])

        Epoch 0025 | Training loss 7.962917 | Training R2 0.828338 | Validation loss 9.609860 | Validation R2 0.774418
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [03:03<00:00,  3.66it/s]
tensor([  4.8900,  45.6167,   9.5987,   0.1051,  -0.9369,  39.9992,   8.5798,
         -0.3131,  -1.5515,  39.4073,   9.3195,  -0.3392,  -2.4984,  37.1201,
          8.8991,  -0.9208,  -3.5922,  35.8086,   8.4388,  -1.9218,  -4.8642,
         33.2721,   7.2729,  -3.1486,  -6.2217,  31.8621,   6.4087,  -4.3224,
         -7.6073,  29.6215,   4.9850,  -5.7174,  -8.7939,  28.9284,   4.8174,
         -6.7392,  -9.6808,   7.2845,  -6.6397, -10.4594,  26.3305,   1.3159,
         -8.2648, -11.1160,  24.3990,  -0.4301,  -9.1898, -11.8479,  21.2692,
         -2.0180,  -9.9808, -12.4354,  18.3305,  -3.3384, -13.0876,  -4.3371,
        -11.5662, -13.8299,  17.7920, -14.3870,  -4.9450, -12.6202, -15.1504],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0026 | Training loss 8.169349 | Training R2 0.819323 | Validation loss 8.430163 | Validation R2 0.826403
        Best loss 8.430163 | Best epoch 0026

100%|##########################################################################| 672/672 [03:01<00:00,  3.71it/s]
tensor([ 6.5499, 48.5983, 15.1371,  3.5329], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0027 | Training loss 6.878480 | Training R2 0.871910 | Validation loss 7.949504 | Validation R2 0.845635
        Best loss 7.949504 | Best epoch 0027

100%|##########################################################################| 672/672 [02:58<00:00,  3.77it/s]
tensor([22.4853, 65.2880, 29.7628, 19.7173, 17.9791, 57.3877, 28.7129, 17.0198,
        16.9415, 26.9971, 16.9828, 63.2698, 30.2553, 16.8464, 63.8235, 30.3975,
        16.6662, 63.3403], grad_fn=<IndexBackward0>)
tensor([54.4230, 51.9620, 17.0410,  7.0369,  2.5077, 43.8090, 17.6270,  3.0059,
         2.5940, 15.3480,  2.6174, 55.5800, 18.3240,  2.6966, 55.2450, 18.2160,
         2.6886, 54.4230])

        Epoch 0028 | Training loss 6.115299 | Training R2 0.898757 | Validation loss 5.728622 | Validation R2 0.919838
        Best loss 5.728622 | Best epoch 0028

100%|##########################################################################| 672/672 [02:53<00:00,  3.86it/s]
tensor([ 9.6481, 86.3610, 29.5480,  5.6376, 78.3233, 26.1667,  6.2007, 78.0224,
        24.1587,  6.6242], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.0520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.0935])

        Epoch 0029 | Training loss 6.373678 | Training R2 0.890021 | Validation loss 7.142794 | Validation R2 0.875375
        Best loss 5.728622 | Best epoch 0028

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
```

```
See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 4 --model 5 --save fold_4 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([2.4257, 5.2958, 5.4951], grad_fn=<IndexBackward0>)
tensor([16.0320, 54.3750, 13.4380])

        Epoch 0001 | Training loss 25.501337 | Training R2 -0.760577 | Validation loss 32.142315 | Validation R2 -1.523621
        Best loss 32.142315 | Best epoch 0001

100%|##########################################################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([10.9708, 16.4202, 16.4284, 16.4365, 16.4447, 16.4853, 16.5342, 16.5586,
        16.5830, 21.8501, 21.9070, 21.9640, 22.0047], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947])

        Epoch 0002 | Training loss 25.554596 | Training R2 -0.767938 | Validation loss 33.443089 | Validation R2 -1.732012
        Best loss 32.142315 | Best epoch 0001

100%|##########################################################################| 672/672 [01:35<00:00,  7.00it/s]
tensor([ 7.0450, 10.0154, 10.0010,  9.9866], grad_fn=<IndexBackward0>)
tensor([21.4040, 31.6970, 25.8410, 21.4040])

        Epoch 0003 | Training loss 24.312588 | Training R2 -0.600264 | Validation loss 32.068600 | Validation R2 -1.512059
        Best loss 32.068600 | Best epoch 0003

100%|##########################################################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 4.0094,  7.7182,  7.1797,  6.7086, 10.2464,  8.3896, 11.8718,  9.6665,
        13.0503, 10.4877, 11.8137, 10.9202, 11.9601], grad_fn=<IndexBackward0>)
tensor([ 2.5158, 10.0050,  2.5792,  0.8070, 40.4740,  0.8047, 40.4720,  0.8047,
        39.6860,  0.7875,  2.5158,  0.7872,  2.5158])

        Epoch 0004 | Training loss 18.267012 | Training R2 0.096633 | Validation loss 19.870958 | Validation R2 0.035488
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 4.8690,  9.7944,  7.7008, 13.1650, 11.7143], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0005 | Training loss 18.761860 | Training R2 0.047026 | Validation loss 21.200550 | Validation R2 -0.097903
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([21.4091, 34.6569, 32.5763], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0006 | Training loss 17.982162 | Training R2 0.124587 | Validation loss 20.414364 | Validation R2 -0.017986
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:31<00:00,  7.38it/s]
tensor([18.8598, 29.9787, 27.4882], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0007 | Training loss 16.927532 | Training R2 0.224260 | Validation loss 19.159618 | Validation R2 0.103307
        Best loss 19.159618 | Best epoch 0007

100%|##########################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([17.9655, 34.3182, 30.5375, 23.3251, 34.3692, 29.5117, 18.7665, 22.5827,
        16.5382, 13.3714, 16.2217, 13.3905, 11.9360, 14.2540, 12.4377, 11.5434,
        13.4844, 12.0562], grad_fn=<IndexBackward0>)
tensor([ 7.2463, 70.3430, 22.7780,  3.3003, 60.2640, 24.0900,  3.4903, 24.0210,
         8.4887,  3.4804, 20.9620,  7.4078,  3.5238, 20.8010,  7.3509,  3.4968,
        20.5050,  7.2463])

        Epoch 0008 | Training loss 16.370752 | Training R2 0.274452 | Validation loss 18.973333 | Validation R2 0.120659
        Best loss 18.973333 | Best epoch 0008

100%|##########################################################################| 672/672 [01:32<00:00,  7.27it/s]
tensor([12.1032, 24.9048, 20.8033, 13.0126, 22.6410, 17.7574,  9.1748,  8.4137,
        14.9725, 11.3985,  7.3387, 11.5282,  9.2648,  7.5464, 10.3042,  9.3327,
         7.9904, 10.2717,  9.5589,  8.7520, 10.6169, 10.2095,  9.4622, 11.3097,
        10.8562, 10.8053, 11.4501, 10.8654, 10.3499, 11.8088, 11.2397, 10.5846,
        11.9419, 10.5950, 11.9133, 11.2289, 10.4416, 11.6993, 10.9565, 10.1020,
        11.3339, 10.4162], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568, 46.7250, 14.1790,  2.9953, 45.9950, 15.9860,
         2.9515, 45.8260, 15.7550,  2.9235, 46.3120, 16.0030,  2.9695, 46.4360,
        16.0330,  2.9750, 20.4610,  7.2470,  2.9262, 21.0770,  8.4980,  3.0144,
        20.5900,  2.9448, 20.6570,  8.3285,  2.9543, 20.5540,  8.2870,  2.9396,
        20.8050,  7.3688])

        Epoch 0009 | Training loss 14.815959 | Training R2 0.405723 | Validation loss 16.785484 | Validation R2 0.311764
        Best loss 16.785484 | Best epoch 0009

100%|##########################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([15.2201, 37.9792, 30.4121, 22.7532, 16.1195, 34.4087, 22.6515],
       grad_fn=<IndexBackward0>)
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0010 | Training loss 14.673149 | Training R2 0.417125 | Validation loss 16.793373 | Validation R2 0.311117
        Best loss 16.785484 | Best epoch 0009

100%|##########################################################################| 672/672 [01:31<00:00,  7.38it/s]
tensor([12.6484, 24.5527,  9.3701, 16.1193,  8.5453, 18.2315, 13.3730,  8.7617],
       grad_fn=<IndexBackward0>)
tensor([23.5920, 20.2570,  2.7573, 21.0380,  2.8637, 70.1770, 21.0260,  2.8620])

        Epoch 0011 | Training loss 13.782256 | Training R2 0.485755 | Validation loss 15.996996 | Validation R2 0.374904
        Best loss 15.996996 | Best epoch 0011

100%|##########################################################################| 672/672 [01:33<00:00,  7.16it/s]
tensor([ 4.0998, 27.8276, 26.2090, 24.5929, 18.1533, 13.3494,  7.2182,  3.3014,
        21.8690, 13.4942,  8.6837], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0012 | Training loss 13.303948 | Training R2 0.520829 | Validation loss 15.555521 | Validation R2 0.408930
        Best loss 15.555521 | Best epoch 0012

100%|##########################################################################| 672/672 [01:32<00:00,  7.27it/s]
tensor([ 9.7279, 32.9579, 31.1551, 27.5726, 20.4980, 15.2696,  8.3477,  2.3601,
        19.6387, 10.3360,  5.2515,  2.0294, 14.1004,  8.3174,  4.3076,  1.9895,
        11.4774,  8.7051,  4.2783,  3.9683, 10.1298,  7.9004,  6.9519,  5.8924,
        11.1614,  9.8574,  8.5018,  7.2632, 12.1099, 10.6808,  9.4548,  8.2704,
        12.6488, 11.3100,  9.9475,  8.7581, 12.8870, 11.5066],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385,
        43.0630, 20.8330,  1.9210,  1.3667, 43.0860,  8.8969,  3.7979,  1.3674,
        42.5380, 12.3470,  3.7496,  1.3500, 42.9850, 10.5230,  3.7888,  1.3642,
        43.0840, 12.5050,  3.7977,  1.3674, 43.0840, 12.5050])

        Epoch 0013 | Training loss 13.012312 | Training R2 0.541607 | Validation loss 15.213802 | Validation R2 0.434613
        Best loss 15.213802 | Best epoch 0013

100%|##########################################################################| 672/672 [01:33<00:00,  7.21it/s]
tensor([ 0.2745, 10.0347,  2.2603, -0.2056, -0.6719,  8.2394,  3.7114,  1.4496,
         1.0090,  8.3221,  4.2308,  2.6189,  2.3726,  7.1274,  5.6220,  4.6618,
         4.4669,  8.3041,  7.0924,  5.9960,  5.8123,  9.2877,  7.8543,  6.7494,
        10.1614,  8.6661,  7.3556, 10.6087,  8.6681,  7.7108, 10.9884,  9.1611,
         7.9981, 11.2231,  9.1500,  8.1591, 11.2712,  9.3742],
       grad_fn=<IndexBackward0>)
tensor([ 5.3298, 14.8900,  5.0763,  2.4483,  2.1161, 14.7070,  5.2983,  2.5554,
         2.2086, 14.9430,  5.3834,  2.5964,  2.2441, 12.6780,  5.2850,  2.5490,
         2.2031, 16.6050,  5.9815,  2.4934,  2.1551, 16.9430,  5.2750,  2.1989,
        19.6280,  6.1089,  2.2010, 19.5260,  4.5398,  2.1895, 19.9330,  5.3619,
         2.2351, 20.0550,  4.6626,  2.2488, 19.8140,  5.3298])

        Epoch 0014 | Training loss 12.533939 | Training R2 0.574691 | Validation loss 14.716722 | Validation R2 0.470956
        Best loss 14.716722 | Best epoch 0014

100%|##########################################################################| 672/672 [01:33<00:00,  7.21it/s]
tensor([ 6.7641, 18.5638,  6.5979, 23.9049, 15.6916], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0015 | Training loss 12.104251 | Training R2 0.603352 | Validation loss 14.334991 | Validation R2 0.498045
        Best loss 14.334991 | Best epoch 0015

100%|##########################################################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([13.9795, 46.5863, 19.0863,  4.8340, 29.5911, 16.0146,  4.8011, 21.8338,
        12.8681,  4.3595], grad_fn=<IndexBackward0>)
tensor([14.0340, 52.5400, 13.3690,  1.8996, 54.8650, 14.0150,  1.9913, 37.1760,
        11.8580,  1.9824])

        Epoch 0016 | Training loss 11.550217 | Training R2 0.638832 | Validation loss 13.747127 | Validation R2 0.538370
        Best loss 13.747127 | Best epoch 0016

100%|##########################################################################| 672/672 [01:34<00:00,  7.11it/s]
tensor([ 4.0921, 18.3844,  3.6786, 16.8184,  5.1207, 14.0996,  5.4195, 14.2547,
         6.1746, 13.5347,  6.7133, 14.0622, 10.0545,  7.3826, 10.5945,  8.0517,
        11.2127,  8.8817, 15.2608, 11.8977,  9.8144, 12.7852, 10.7657, 13.3178,
        11.8928, 11.6402, 14.6168, 12.6066, 15.4988, 13.4973],
       grad_fn=<IndexBackward0>)
tensor([ 2.9329, 18.1390,  2.8114, 19.1060,  2.9618, 16.6620,  2.9542, 19.3020,
         2.9922, 19.2630,  2.9861, 19.0680,  7.4988,  2.9560,  7.4813,  2.9491,
         7.4269,  2.9277, 19.0190,  7.4794,  2.9484,  7.5152,  2.9625,  6.4918,
         3.3388,  2.9231,  7.5188,  2.9639,  7.4401,  2.9329])

        Epoch 0017 | Training loss 11.089778 | Training R2 0.667053 | Validation loss 13.340640 | Validation R2 0.565266
        Best loss 13.340640 | Best epoch 0017

100%|##########################################################################| 672/672 [01:35<00:00,  7.03it/s]
tensor([16.4245, 59.1090, 21.8380], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0018 | Training loss 10.320528 | Training R2 0.711641 | Validation loss 11.873363 | Validation R2 0.655636
        Best loss 11.873363 | Best epoch 0018
```

```
100%|##########################################################################| 672/672 [01:36<00:00,  6.98it/s]
tensor([17.6073, 63.8990, 24.1658,  5.6614, 44.2576, 22.5470,  6.5664],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444])

        Epoch 0019 | Training loss 9.479305 | Training R2 0.756734 | Validation loss 11.307576 | Validation R2 0.687673
        Best loss 11.307576 | Best epoch 0019

100%|##########################################################################| 672/672 [01:38<00:00,  6.83it/s]
tensor([22.7205, 66.8948, 26.8823, 15.5828], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0020 | Training loss 8.340364 | Training R2 0.811679 | Validation loss 8.864890 | Validation R2 0.808037
        Best loss 8.864890 | Best epoch 0020

100%|##########################################################################| 672/672 [01:41<00:00,  6.59it/s]
tensor([10.0821, 26.9367, 20.8400, 17.0122, 11.5361, 15.8813, 36.3308, 25.5300,
        17.7422, 30.3660, 18.7054, 27.2397, 19.3506, 30.3209, 19.6491],
       grad_fn=<IndexBackward0>)
tensor([20.9330, 26.7620, 22.9870, 19.9020, 13.0070, 17.6410, 46.8390, 29.5720,
        19.3340, 35.8980, 20.3400, 31.7000, 20.7250, 36.8060, 20.8550])

        Epoch 0021 | Training loss 7.650942 | Training R2 0.841526 | Validation loss 8.756156 | Validation R2 0.812718
        Best loss 8.756156 | Best epoch 0021

100%|##########################################################################| 672/672 [01:47<00:00,  6.25it/s]
tensor([ 3.7586, 33.9919,  8.2549,  1.2967, -1.8662, -2.1911, 12.2417,  1.5280,
        -1.5885, -1.8975, 11.5778,  2.3445, -1.2041, -1.4682],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0022 | Training loss 6.915258 | Training R2 0.870537 | Validation loss 6.888650 | Validation R2 0.884085
        Best loss 6.888650 | Best epoch 0022

100%|##########################################################################| 672/672 [02:03<00:00,  5.44it/s]
tensor([ 1.5398,  4.4927,  3.3403,  2.5443,  1.9098,  0.1433, -0.4094, -0.6202,
        -0.6513, -0.6544,  2.8599, -0.0619, -0.3231, -0.5211, -0.5408,  2.8718,
         0.0123, -0.4279, -0.4479], grad_fn=<IndexBackward0>)
tensor([0.1027, 4.3675, 3.3207, 2.6789, 2.2198, 1.1160, 0.6726, 0.3426, 0.2066,
        0.1245, 4.4427, 1.1442, 0.8164, 0.3513, 0.1277, 4.4458, 1.1451, 0.3516,
        0.1278])

        Epoch 0023 | Training loss 6.409317 | Training R2 0.888788 | Validation loss 6.464874 | Validation R2 0.897908
        Best loss 6.464874 | Best epoch 0023

100%|##########################################################################| 672/672 [02:22<00:00,  4.72it/s]
tensor([ 9.2943, 67.5948, 20.8247,  3.1299, 21.1432,  4.3623, 20.8246,  4.6365,
        21.1392,  5.1836], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0024 | Training loss 6.434866 | Training R2 0.887899 | Validation loss 6.995244 | Validation R2 0.880470
        Best loss 6.464874 | Best epoch 0023

100%|##########################################################################| 672/672 [02:31<00:00,  4.44it/s]
tensor([ 7.0800, 75.9345, 57.3135, 47.6548, 39.5218, 14.2651,  2.0937, -0.6384,
        -2.3179, 56.9519, 15.1308,  2.2615, -1.8054, 57.1468, 16.1390,  3.2208,
         0.1911], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947, 73.8930, 26.4440, 10.0160,
         5.0069])

        Epoch 0025 | Training loss 6.013347 | Training R2 0.902105 | Validation loss 6.196391 | Validation R2 0.906212
        Best loss 6.196391 | Best epoch 0025

100%|##########################################################################| 672/672 [02:39<00:00,  4.21it/s]
tensor([24.2445, 61.1039], grad_fn=<IndexBackward0>)
tensor([47.8150, 46.0380])

        Epoch 0026 | Training loss 6.441009 | Training R2 0.887685 | Validation loss 5.943230 | Validation R2 0.913719
        Best loss 5.943230 | Best epoch 0026

100%|##########################################################################| 672/672 [02:41<00:00,  4.16it/s]
tensor([20.4664, 65.3887, 21.7751], grad_fn=<IndexBackward0>)
tensor([28.6530, 67.5770, 24.1020])

        Epoch 0027 | Training loss 6.147571 | Training R2 0.897686 | Validation loss 5.676152 | Validation R2 0.921299
        Best loss 5.676152 | Best epoch 0027

100%|##########################################################################| 672/672 [02:39<00:00,  4.21it/s]
tensor([ 5.5889, 51.8624, 13.1392,  2.6198], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0028 | Training loss 6.355262 | Training R2 0.890656 | Validation loss 5.838716 | Validation R2 0.916727
        Best loss 5.676152 | Best epoch 0027

100%|##########################################################################| 672/672 [02:42<00:00,  4.12it/s]
tensor([10.5076, 63.3576, 17.9138,  3.0357, 61.1687, 18.1363,  3.4611, 61.1664,
        17.9986,  5.9321,  3.2432], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])

        Epoch 0029 | Training loss 6.041739 | Training R2 0.901178 | Validation loss 5.606994 | Validation R2 0.923206
        Best loss 5.606994 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 5 --model 1 --save fold_5 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([2.1999, 5.6524, 5.8418, 6.1936, 9.4868, 9.8432],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521])

        Epoch 0001 | Training loss 24.587435 | Training R2 -0.636649 | Validation loss 29.936550 | Validation R2 -1.189140
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:33<00:00,  7.22it/s]
tensor([ 4.9043,  8.9507,  9.0836,  9.2166,  9.3305, 13.3845, 13.5179, 13.6512,
        13.7654, 17.8186, 17.9522, 18.0858], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243, 63.0070, 16.7890,  4.7756])

        Epoch 0002 | Training loss 25.483650 | Training R2 -0.758136 | Validation loss 33.067993 | Validation R2 -1.671072
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 7.6014, 11.0011, 11.0285], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0003 | Training loss 24.522160 | Training R2 -0.627971 | Validation loss 32.016544 | Validation R2 -1.503911
        Best loss 29.936550 | Best epoch 0001

100%|##########################################################################| 672/672 [01:32<00:00,  7.23it/s]
tensor([ 7.3291, 10.1608, 10.0233,  9.8829], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0004 | Training loss 22.401255 | Training R2 -0.358544 | Validation loss 28.629280 | Validation R2 -1.002123
        Best loss 28.629280 | Best epoch 0004

100%|##########################################################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([14.4474, 19.8099, 19.4276, 18.6136, 23.0821, 21.7736, 26.9981, 26.1418,
        24.3684, 28.5206, 26.5152], grad_fn=<IndexBackward0>)
tensor([20.1800, 76.4000, 23.3070,  3.2069, 20.8640,  3.3441, 78.8070, 24.2140,
         3.3317, 23.8640,  3.2836])

        Epoch 0005 | Training loss 19.169922 | Training R2 0.005122 | Validation loss 21.290998 | Validation R2 -0.107291
        Best loss 21.290998 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([12.2309, 18.9201, 18.0805, 16.3241, 20.7797, 18.8313, 22.8460, 20.6343,
        24.4485, 21.9717], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0006 | Training loss 19.678331 | Training R2 -0.048349 | Validation loss 22.492300 | Validation R2 -0.235770
        Best loss 21.290998 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([ 9.0321, 16.7148, 15.5704, 14.4203], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0007 | Training loss 18.438383 | Training R2 0.079604 | Validation loss 20.871935 | Validation R2 -0.064132
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([ 0.2794,  0.7751,  0.5484, -0.3596, -1.0415, -1.9520, -2.6358, -3.3204,
        -2.3768, -4.0057, -5.6395], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0008 | Training loss 20.370321 | Training R2 -0.123375 | Validation loss 23.957869 | Validation R2 -0.402059
```

```
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([17.7417, 27.3907, 25.9303], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0009 | Training loss 19.084763 | Training R2 0.013942 | Validation loss 21.900980 | Validation R2 -0.171647
        Best loss 20.871935 | Best epoch 0007

100%|##########################################################################| 672/672 [01:31<00:00,  7.36it/s]
tensor([17.3056, 25.6101, 24.2517, 20.7280, 26.5591, 24.9605, 21.8946, 26.8496,
        25.2540, 22.2393], grad_fn=<IndexBackward0>)
tensor([17.8830, 55.3190, 16.9870,  2.1271, 56.8470, 17.5230,  2.1942, 57.7130,
        17.7900,  2.2277])

        Epoch 0010 | Training loss 17.859404 | Training R2 0.136499 | Validation loss 20.114540 | Validation R2 0.011697
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([ 8.7530, 19.8132, 16.8510, 16.2882, 22.7456, 19.5403, 19.2723],
       grad_fn=<IndexBackward0>)
tensor([ 9.2660, 25.5950,  5.0055,  3.7205, 26.2690,  4.4291,  3.8185])

        Epoch 0011 | Training loss 18.237335 | Training R2 0.099566 | Validation loss 20.373814 | Validation R2 -0.013945
        Best loss 20.114540 | Best epoch 0010

100%|##########################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([ 9.9975, 15.6876, 13.4450, 11.2903, 17.1275, 15.1765, 11.2384],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727])

        Epoch 0012 | Training loss 17.548340 | Training R2 0.166316 | Validation loss 19.443098 | Validation R2 0.076577
        Best loss 19.443098 | Best epoch 0012

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([ 9.9177, 18.4395, 17.9721, 17.5216, 14.3823, 12.5939, 11.2551,  9.9186,
        16.4753, 13.0464], grad_fn=<IndexBackward0>)
tensor([ 4.1835, 35.5470, 29.2780, 24.3620,  6.9018,  3.3599,  1.9581,  1.1412,
        14.7460,  4.1835])

        Epoch 0013 | Training loss 17.206947 | Training R2 0.198439 | Validation loss 19.141432 | Validation R2 0.105009
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([12.4364, 27.2565, 23.2694, 19.6116, 16.4919, 29.9886, 27.1892, 23.8359,
        20.2024], grad_fn=<IndexBackward0>)
tensor([ 4.7756, 60.3880, 16.0390,  4.5623,  1.5531, 62.9590, 16.7740,  4.7714,
         1.6243])

        Epoch 0014 | Training loss 17.306837 | Training R2 0.189105 | Validation loss 19.362793 | Validation R2 0.084189
        Best loss 19.141432 | Best epoch 0013

100%|##########################################################################| 672/672 [01:31<00:00,  7.32it/s]
tensor([ 9.0598, 20.0499, 19.4907, 18.9320, 17.8166, 16.1479, 12.2752, 10.0752,
         8.9788, 18.8787, 14.2877, 10.3545,  8.6562, 18.4221, 14.3182, 10.7028,
         9.1701], grad_fn=<IndexBackward0>)
tensor([ 1.7205, 44.8430, 33.8580, 27.3170, 18.5670, 10.6030,  2.8810,  1.3684,
         0.9431, 27.6900,  6.1533,  1.6721,  0.9567, 23.0698,  6.2359,  1.6946,
         0.9695])

        Epoch 0015 | Training loss 16.755896 | Training R2 0.239911 | Validation loss 19.031542 | Validation R2 0.115256
        Best loss 19.031542 | Best epoch 0015

100%|##########################################################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([  0.9582,   1.0904,   0.4565,  -1.8299,  -3.4424,  -5.5529,  -7.1404,
         -8.7248,  -7.3052, -10.9318, -14.4289], grad_fn=<IndexBackward0>)
tensor([0.2320, 4.0372, 3.1668, 1.2218, 0.5990, 0.2316, 0.1136, 0.0557, 7.0164,
        1.2240, 0.2320])

        Epoch 0016 | Training loss 16.645119 | Training R2 0.249928 | Validation loss 18.393700 | Validation R2 0.173566
        Best loss 18.393700 | Best epoch 0016

100%|##########################################################################| 672/672 [01:35<00:00,  7.07it/s]
tensor([ 6.8242, 20.9803, 15.5757, 10.6441,  6.5071, 20.2602, 15.3891, 10.3295,
         6.6992, 19.2614, 16.2280, 12.1368,  8.1876], grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581])

        Epoch 0017 | Training loss 16.093096 | Training R2 0.298854 | Validation loss 17.970434 | Validation R2 0.211163
        Best loss 17.970434 | Best epoch 0017

100%|##########################################################################| 672/672 [01:40<00:00,  6.72it/s]
tensor([12.8932, 35.1585, 29.2565, 17.6236, 35.2379, 31.1231, 21.2395],
       grad_fn=<IndexBackward0>)
tensor([ 3.8765, 62.3080, 16.2100,  1.3937, 63.5960, 16.5530,  1.4231])

        Epoch 0018 | Training loss 15.311383 | Training R2 0.365315 | Validation loss 16.984724 | Validation R2 0.295328
        Best loss 16.984724 | Best epoch 0018

100%|##########################################################################| 672/672 [01:51<00:00,  6.03it/s]
tensor([16.5482, 29.7475, 28.0376], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0019 | Training loss 14.230635 | Training R2 0.451751 | Validation loss 15.854136 | Validation R2 0.386019
        Best loss 15.854136 | Best epoch 0019

100%|##########################################################################| 672/672 [02:03<00:00,  5.43it/s]
tensor([19.7466, 42.1145, 30.2606, 14.1118, 37.6893, 25.5962, 11.4744, 34.7414,
        11.2551, 33.2510, 23.2312, 11.2077, 33.0895, 23.2144, 11.2046, 32.8959,
        23.1463, 11.2140, 32.9500, 23.3397, 11.3844, 32.9221, 23.4265, 11.5103,
        23.5826, 11.6663, 32.9310, 23.6521, 11.7840, 32.9144, 23.7639],
       grad_fn=<IndexBackward0>)
tensor([19.8480, 53.1050, 18.5150,  3.2922, 56.7650, 19.9680,  3.5506, 57.2050,
         3.5796, 56.8250, 19.9970,  3.5558, 56.6030, 19.9170,  3.5416, 56.1670,
        19.7650,  3.5145, 56.5720, 19.9040,  3.5392, 56.4240, 19.8470,  3.5291,
        19.8520,  3.5300, 56.3440, 19.8300,  3.5261, 56.4400, 19.8480])

        Epoch 0020 | Training loss 12.025496 | Training R2 0.608497 | Validation loss 13.721763 | Validation R2 0.540072
        Best loss 13.721763 | Best epoch 0020

100%|##########################################################################| 672/672 [02:27<00:00,  4.56it/s]
tensor([11.1434, 49.1650, 25.8507, 12.7483], grad_fn=<IndexBackward0>)
tensor([ 0.4385, 64.0190, 10.8380,  2.4664])

        Epoch 0021 | Training loss 12.230107 | Training R2 0.595061 | Validation loss 13.446256 | Validation R2 0.558356
        Best loss 13.446256 | Best epoch 0021

100%|##########################################################################| 672/672 [02:41<00:00,  4.15it/s]
tensor([ 7.8498, 35.5636, 31.8140, 27.4297, 23.8189, 15.3497, 39.8910, 28.7233,
        18.5893, 41.6949, 30.8928, 19.8995, 41.8754, 38.6326, 20.1299, 38.6822,
        20.5340, 38.5935, 21.5521], grad_fn=<IndexBackward0>)
tensor([12.5700, 31.8440, 25.2520, 20.7650, 17.3880, 10.5840, 40.6760, 22.8730,
        13.9690, 43.5540, 24.6480, 15.0630, 44.0460, 35.6960, 15.2700, 35.8460,
        15.3380, 35.8950, 15.3590])

        Epoch 0022 | Training loss 9.790716 | Training R2 0.740488 | Validation loss 12.751149 | Validation R2 0.602837
        Best loss 12.751149 | Best epoch 0022

100%|##########################################################################| 672/672 [02:39<00:00,  4.22it/s]
tensor([14.1666, 61.5551, 29.6613,  8.8076, 58.5753, 24.2845,  8.8832],
       grad_fn=<IndexBackward0>)
tensor([ 6.2430, 65.8400, 25.1060,  4.2933, 69.2210, 23.5690,  4.5781])

        Epoch 0023 | Training loss 8.497423 | Training R2 0.804519 | Validation loss 10.855521 | Validation R2 0.712147
        Best loss 10.855521 | Best epoch 0023

100%|##########################################################################| 672/672 [02:46<00:00,  4.03it/s]
tensor([15.8495, 61.9667, 28.1483, 10.4488], grad_fn=<IndexBackward0>)
tensor([18.4370, 63.6710, 21.1850,  2.2930])

        Epoch 0024 | Training loss 7.026572 | Training R2 0.866335 | Validation loss 7.219308 | Validation R2 0.872690
        Best loss 7.219308 | Best epoch 0024

100%|##########################################################################| 672/672 [03:05<00:00,  3.62it/s]
tensor([15.0177, 53.2453, 22.2480, 13.1297, 52.0899, 24.2600],
       grad_fn=<IndexBackward0>)
tensor([20.1680, 53.7810, 19.0680,  3.5221, 56.3060, 20.1680])

        Epoch 0025 | Training loss 22.096283 | Training R2 -0.321805 | Validation loss 31.622337 | Validation R2 -1.442631
        Best loss 7.219308 | Best epoch 0024

100%|##########################################################################| 672/672 [03:00<00:00,  3.71it/s]
tensor([ 9.0573, 64.0458, 19.9370,  7.2607,  4.3328, 59.8810, 18.9035,  3.8537],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0026 | Training loss 6.403774 | Training R2 0.888980 | Validation loss 6.044273 | Validation R2 0.910760
        Best loss 6.044273 | Best epoch 0026

100%|##########################################################################| 672/672 [02:59<00:00,  3.74it/s]
tensor([ 6.9223, 61.5160, 18.7082,  3.0362, 18.1905,  2.9401, 18.2441,  2.8033],
       grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559])

        Epoch 0027 | Training loss 6.205529 | Training R2 0.895747 | Validation loss 6.115032 | Validation R2 0.908659
        Best loss 6.044273 | Best epoch 0026

100%|##########################################################################| 672/672 [03:01<00:00,  3.70it/s]
tensor([ 6.6950, 60.9784, 50.3774, 41.8519, 28.7659, 16.2084,  8.8678,  3.7320,
         2.6390], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0028 | Training loss 6.358976 | Training R2 0.890528 | Validation loss 5.888662 | Validation R2 0.915296
        Best loss 5.888662 | Best epoch 0028

100%|##########################################################################| 672/672 [02:59<00:00,  3.74it/s]
tensor([ 5.4355, 52.7556, 12.8180,  2.5391], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])
```

```
        Epoch 0029 | Training loss 6.320073 | Training R2 0.891863 | Validation loss 5.790334 | Validation R2 0.918101
        Best loss 5.790334 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 5 --model 2 --save fold_5 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([ 2.8724,  6.5957,  6.8080,  6.9899,  7.2021, 10.7213, 10.9348, 11.3314,
        14.8272, 15.0422, 15.1036, 15.4413, 18.9374, 19.1537, 19.5554, 23.0516,
        23.2693, 23.6736, 27.3578, 27.6082, 27.7960, 30.7728, 30.9930, 31.2133],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666,
        61.4260, 21.6510, 16.6580,  3.9438, 61.4060, 21.6430,  3.9424, 61.4240,
        21.6460,  3.9429, 24.6850,  8.6517,  3.9430, 52.7138, 18.6040,  7.4356])

        Epoch 0001 | Training loss 25.439198 | Training R2 -0.752008 | Validation loss 31.925747 | Validation R2 -1.489729
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([ 3.2931,  5.3593,  5.3786,  5.3980,  5.4173,  5.4752,  7.2988,  7.3569,
         7.4149,  9.1766,  9.2347,  9.2928, 11.0515, 11.1676, 12.9117, 13.0278,
        14.7861, 14.9023, 16.6606, 16.7768, 18.5066, 18.6228, 20.3668, 20.4830,
        22.2271, 22.3433, 24.1067, 24.2035, 25.9476, 26.0638, 27.7936, 27.9099,
        29.6397, 29.7559, 31.4857, 31.6020, 33.4481, 35.1973, 35.2942, 37.0240,
        37.1403, 38.8701, 38.9864, 40.7162, 40.8325, 42.5338, 42.6501, 44.3800,
        44.4963, 46.1862, 46.2250], grad_fn=<IndexBackward0>)
tensor([13.4790, 18.8570, 13.8900, 10.7480,  8.5627,  4.6489, 22.6090, 10.6930,
         5.8463, 23.2430, 11.0850,  6.0691, 23.4230,  6.1265, 23.3150,  6.1035,
        23.4510,  6.1355, 23.4760,  6.1434, 23.1780,  6.0705, 23.2750,  6.0899,
        23.2850,  6.0940, 17.6110,  6.0951, 23.2930,  6.0960, 23.1390,  6.0582,
        23.1120,  6.0491, 23.1050,  6.0467,  6.0455, 17.4690,  6.0458, 23.1040,
         6.0462, 23.0980,  6.0454, 23.0970,  6.0451, 22.8050,  5.9719, 23.0390,
         6.0265, 22.6590, 13.4790])

        Epoch 0002 | Training loss 26.376934 | Training R2 -0.883553 | Validation loss 34.834122 | Validation R2 -1.964010
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################| 672/672 [01:30<00:00,  7.47it/s]
tensor([ 7.8250, 11.8784, 11.8799, 11.8814, 11.8873, 11.8917, 11.8975, 11.9019,
        11.9062, 15.7652, 15.7763, 15.7875], grad_fn=<IndexBackward0>)
tensor([ 2.8854, 42.8980, 34.5060, 27.9840, 12.2340,  6.5823,  2.8806,  1.5499,
         0.8339, 54.9410, 12.2540,  2.8854])

        Epoch 0003 | Training loss 24.805820 | Training R2 -0.665852 | Validation loss 32.632885 | Validation R2 -1.601243
        Best loss 31.925747 | Best epoch 0001

100%|##########################################################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([ 8.7386, 11.7069, 11.5418, 11.3754, 11.2797, 11.2316, 13.9237, 13.7604,
        13.6669, 13.6202, 16.3320, 16.2147, 16.1207, 16.0738],
       grad_fn=<IndexBackward0>)
tensor([ 5.1825, 48.9670, 16.9790,  6.3620,  3.6307,  2.7427, 18.1490,  6.8804,
         3.8809,  2.9318, 14.1770,  7.0320,  4.0131,  3.0316])

        Epoch 0004 | Training loss 22.594074 | Training R2 -0.382033 | Validation loss 29.154833 | Validation R2 -1.076304
        Best loss 29.154833 | Best epoch 0004

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([13.8576, 17.9291, 17.4015, 16.8603], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0005 | Training loss 19.321512 | Training R2 -0.010675 | Validation loss 21.662233 | Validation R2 -0.146242
        Best loss 21.662233 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([11.5918, 16.2894, 16.0552], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5668])

        Epoch 0006 | Training loss 18.806362 | Training R2 0.042500 | Validation loss 20.810762 | Validation R2 -0.057903
        Best loss 20.810762 | Best epoch 0006

100%|##########################################################################| 672/672 [01:30<00:00,  7.46it/s]
tensor([13.7967, 24.9147, 23.5840, 22.4126, 21.0541, 27.8658, 26.2462, 23.2119],
       grad_fn=<IndexBackward0>)
tensor([ 7.4356, 60.5650, 21.1270,  9.6255,  3.8483, 61.8760, 21.7760,  3.9666])

        Epoch 0007 | Training loss 18.502975 | Training R2 0.073144 | Validation loss 20.257120 | Validation R2 -0.002364
        Best loss 20.257120 | Best epoch 0007

100%|##########################################################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 7.3947, 16.2876, 14.5021], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0008 | Training loss 17.884424 | Training R2 0.134077 | Validation loss 19.712755 | Validation R2 0.050785
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([ 7.4039, 16.9333, 14.2522], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0009 | Training loss 18.018396 | Training R2 0.121056 | Validation loss 20.877218 | Validation R2 -0.064670
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:30<00:00,  7.43it/s]
tensor([0.6249, 7.8101, 7.3241, 3.8194, 1.0698], grad_fn=<IndexBackward0>)
tensor([0.1817, 6.2759, 4.8730, 0.8292, 0.1817])

        Epoch 0010 | Training loss 17.464170 | Training R2 0.174295 | Validation loss 20.522924 | Validation R2 -0.028841
        Best loss 19.712755 | Best epoch 0008

100%|##########################################################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 9.3226, 15.8665,  8.5315, 13.2728,  7.9733], grad_fn=<IndexBackward0>)
tensor([15.8300, 13.0430,  1.2608, 15.9120,  1.2850])

        Epoch 0011 | Training loss 15.910845 | Training R2 0.314645 | Validation loss 18.198824 | Validation R2 0.190985
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################| 672/672 [01:31<00:00,  7.35it/s]
tensor([ 4.3449, 16.5067], grad_fn=<IndexBackward0>)
tensor([ 2.4489, 16.6950])

        Epoch 0012 | Training loss 15.860810 | Training R2 0.318949 | Validation loss 18.750023 | Validation R2 0.141237
        Best loss 18.198824 | Best epoch 0011

100%|##########################################################################| 672/672 [01:32<00:00,  7.28it/s]
tensor([ 8.7084, 25.3828, 17.3558,  9.8191,  3.7226,  1.3463, 10.4619,  6.1137,
         2.9816, 10.1290,  7.5545,  4.8109,  4.4536], grad_fn=<IndexBackward0>)
tensor([ 7.2829, 42.8440, 12.3400,  4.1313,  1.6174,  1.6724, 20.9970,  5.9940,
         1.7166, 17.7690,  5.9424,  1.9898,  1.7019])

        Epoch 0013 | Training loss 13.904661 | Training R2 0.476580 | Validation loss 15.886896 | Validation R2 0.383479
        Best loss 15.886896 | Best epoch 0013

100%|##########################################################################| 672/672 [01:33<00:00,  7.20it/s]
tensor([ 7.0433, 27.5600, 16.8307,  7.2308,  0.1864,  9.9691,  3.3722, -0.6687,
         7.9056,  3.2674, -0.1207], grad_fn=<IndexBackward0>)
tensor([ 1.7436, 45.8730, 13.5250,  4.4589,  1.7225, 16.4400,  5.4192,  1.7866,
        16.0580,  5.2932,  1.7451])

        Epoch 0014 | Training loss 12.929752 | Training R2 0.547405 | Validation loss 15.179044 | Validation R2 0.437194
        Best loss 15.179044 | Best epoch 0014

100%|##########################################################################| 672/672 [01:34<00:00,  7.09it/s]
tensor([ 7.4332, 30.5729, 16.2396], grad_fn=<IndexBackward0>)
tensor([ 0.9012, 40.1090, 10.2340])

        Epoch 0015 | Training loss 12.248608 | Training R2 0.593835 | Validation loss 14.446182 | Validation R2 0.490228
        Best loss 14.446182 | Best epoch 0015

100%|##########################################################################| 672/672 [01:35<00:00,  7.06it/s]
tensor([ 4.6836,  7.6980,  7.1804, 17.4322, 10.2643,  9.2034, 19.8746, 11.5507,
        10.7448, 13.1053, 12.3932, 20.9605, 14.0527, 22.7131, 18.8298],
       grad_fn=<IndexBackward0>)
tensor([ 8.4665,  2.6608,  2.2691, 18.5760,  3.2225,  2.3435, 25.5770,  3.2261,
         2.3462,  3.2262,  2.3463, 25.6730,  2.3549, 30.2890,  8.4665])

        Epoch 0016 | Training loss 11.735577 | Training R2 0.627147 | Validation loss 14.173969 | Validation R2 0.509258
        Best loss 14.173969 | Best epoch 0016

100%|##########################################################################| 672/672 [01:36<00:00,  6.93it/s]
tensor([11.6500, 60.2137, 25.1021, 10.0511], grad_fn=<IndexBackward0>)
tensor([ 5.7740, 65.1420, 19.1870,  6.7725])

        Epoch 0017 | Training loss 10.962422 | Training R2 0.674656 | Validation loss 14.000322 | Validation R2 0.521209
        Best loss 14.000322 | Best epoch 0017

100%|##########################################################################| 672/672 [01:43<00:00,  6.52it/s]
tensor([ 1.9511, 20.6897,  3.2896, -2.9803, -5.5958, 20.0863,  5.9632, -0.5994,
        -4.8749, 19.8183,  6.0784, -1.1292, -4.3055, 19.2795,  7.1646,  0.7781,
        -3.7093], grad_fn=<IndexBackward0>)
tensor([ 0.1465, 23.7240,  3.6820,  0.5996,  0.1266, 35.6020,  5.5289,  1.1669,
         0.1900, 35.4880,  5.5170,  0.8985,  0.1896, 35.4880,  7.1499,  1.5090,
```

```
         0.1896])

        Epoch 0018 | Training loss 8.945731 | Training R2 0.783349 | Validation loss 10.094747 | Validation R2 0.751079
        Best loss 10.094747 | Best epoch 0018

100%|##########################################################################| 672/672 [02:03<00:00,  5.45it/s]
tensor([18.3829, 63.2539, 23.4179,  4.5281, 46.1589, 19.9410,  4.2955, 35.4959,
        16.3430,  3.1342, 26.7132, 12.0767,  3.3039,  2.6298],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444, 57.7000,
        16.2380,  1.6738, 44.0250, 12.3930,  1.8120,  1.2775])

        Epoch 0019 | Training loss 8.820597 | Training R2 0.789368 | Validation loss 9.154214 | Validation R2 0.795303
        Best loss 9.154214 | Best epoch 0019

100%|##########################################################################| 672/672 [02:18<00:00,  4.85it/s]
tensor([ 4.1644, 14.0128, -0.3138, 27.2210, 10.2752, -0.3314, 23.0703,  7.9699,
        -0.3345], grad_fn=<IndexBackward0>)
tensor([ 1.7265, 18.3160,  2.4943, 49.3870, 15.7180,  2.1405, 40.9940, 12.9500,
         1.7635])

        Epoch 0020 | Training loss 7.317793 | Training R2 0.855026 | Validation loss 7.885971 | Validation R2 0.848092
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:28<00:00,  4.52it/s]
tensor([ 8.4705, 47.7004, 13.9731,  1.0199, 41.2189, 11.3355,  1.4946, 40.8871,
        13.6375,  2.4164, 39.6342, 12.4571,  3.1625], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0021 | Training loss 7.042254 | Training R2 0.865738 | Validation loss 8.384834 | Validation R2 0.828265
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:34<00:00,  4.36it/s]
tensor([ 4.4215, 36.0008,  8.1078,  0.6668, -1.3523, -1.4276, 11.2206, -0.1053,
        -1.8685, -1.9566,  9.4959, -0.7273, -2.5235, -2.5964,  8.4442, -2.1228,
        -3.3086, -3.3706], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307])

        Epoch 0022 | Training loss 9.585545 | Training R2 0.751250 | Validation loss 10.479862 | Validation R2 0.731724
        Best loss 7.885971 | Best epoch 0020

100%|##########################################################################| 672/672 [02:35<00:00,  4.32it/s]
tensor([ 7.7273, 48.1425, 12.7922,  1.4126, 44.4121, 10.8110,  1.8589, 44.7639,
        13.0078,  1.6967, 44.0305, 10.4389,  1.3453], grad_fn=<IndexBackward0>)
tensor([ 2.9463, 47.9160, 16.4030,  2.7094, 51.2510, 15.3770,  2.9173, 52.6370,
        18.1500,  2.9979, 52.4890, 15.7600,  2.9900])

        Epoch 0023 | Training loss 6.300526 | Training R2 0.892531 | Validation loss 5.878633 | Validation R2 0.915584
        Best loss 5.878633 | Best epoch 0023

100%|##########################################################################| 672/672 [02:38<00:00,  4.25it/s]
tensor([ 4.2463, 36.7811,  8.6615,  1.4889, -0.0500, -0.0957, 12.9539,  1.7627,
         0.3970,  0.3455, 12.1383,  1.8436,  0.3857,  0.3445, 11.9547,  1.1080,
         0.2285,  0.1806, 11.7720,  1.7816,  0.1001,  7.4648,  1.6911,  0.0825,
        11.4667,  0.7494, -0.1261, -0.1730,  0.2474, -0.3031, 30.3681,  6.5845,
         0.4806, -0.2833], grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322, 10.7820,  1.6812,
         0.4172,  0.3307, 10.7730,  2.1190,  0.3304,  6.7693,  2.1190,  0.3304,
        10.7810,  1.6811,  0.4171,  0.3307,  1.0556,  0.3304, 35.8960,  6.7693,
         1.3316,  0.4168])

        Epoch 0024 | Training loss 6.111111 | Training R2 0.898896 | Validation loss 5.680680 | Validation R2 0.921174
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:43<00:00,  4.12it/s]
tensor([ 8.8150, 11.5567,  4.6076, 11.2782,  5.0257,  6.5838,  5.3709, 11.5210,
         5.6812, 11.6247,  5.9075, 11.7576,  6.1699, 12.0414,  6.4387, 12.2436],
       grad_fn=<IndexBackward0>)
tensor([14.5460, 14.3260,  2.1336, 15.1440,  2.2555,  7.1526,  2.2158, 14.6630,
         2.1838, 14.4490,  2.1519, 14.3450,  2.1365, 14.4340,  2.1497, 14.5460])

        Epoch 0025 | Training loss 6.472453 | Training R2 0.886586 | Validation loss 7.626081 | Validation R2 0.857940
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:50<00:00,  3.95it/s]
tensor([ 1.5432,  6.2264,  4.7043,  3.4637,  1.7148,  0.1873, -0.2482, -0.3312,
        -0.3259], grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0026 | Training loss 6.822579 | Training R2 0.873984 | Validation loss 8.459892 | Validation R2 0.825177
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:52<00:00,  3.89it/s]
tensor([12.3268, 41.0046, 31.4636], grad_fn=<IndexBackward0>)
tensor([21.0100, 30.1650, 21.5660])

        Epoch 0027 | Training loss 6.095839 | Training R2 0.899400 | Validation loss 6.896765 | Validation R2 0.883812
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [02:50<00:00,  3.95it/s]
tensor([ 3.3598, 38.0550, 32.1865, 26.7041, 11.2778,  5.3198,  1.1977, -0.6329,
        44.5308, 10.9635,  1.2176], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0028 | Training loss 6.544991 | Training R2 0.884030 | Validation loss 6.196602 | Validation R2 0.906206
        Best loss 5.680680 | Best epoch 0024

100%|##########################################################################| 672/672 [03:17<00:00,  3.41it/s]
tensor([ 5.3302, 57.8313, 14.6693,  3.2426,  1.1091, 15.5492,  4.6520,  2.3154,
        58.9204, 16.3087,  2.9490,  2.4515, 56.6236, 16.2949,  5.9694,  2.6612,
        20.1659,  6.1725,  3.0380, 20.9118,  6.8515,  3.4699],
       grad_fn=<IndexBackward0>)
tensor([ 0.8310, 59.4470, 12.7970,  2.9511,  0.8392, 12.6360,  2.9139,  0.8286,
        58.9270, 12.7180,  1.5640,  0.8341, 56.6760, 12.2320,  3.4784,  0.8022,
        15.3490,  3.5396,  0.8163, 15.6260,  3.6034,  0.8310])

        Epoch 0029 | Training loss 6.115059 | Training R2 0.898765 | Validation loss 7.040408 | Validation R2 0.878922
        Best loss 5.680680 | Best epoch 0024

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 5 --model 3 --save fold_5 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 2.0993,  4.3603,  4.5242,  4.8280,  6.9204,  7.1301,  7.3631,  9.4930,
         9.6565,  9.9135, 12.0199, 12.2073, 12.4649], grad_fn=<IndexBackward0>)
tensor([ 7.1280, 48.3090, 16.0790,  2.5997, 40.2000, 10.9370,  2.6928, 34.4200,
        12.7210,  2.7225, 40.6640, 12.7280,  2.7241])

        Epoch 0001 | Training loss 24.240671 | Training R2 -0.590810 | Validation loss 29.148003 | Validation R2 -1.075331
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.60it/s]
tensor([4.3878, 7.2371, 7.3457], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0002 | Training loss 25.267263 | Training R2 -0.728405 | Validation loss 32.724815 | Validation R2 -1.615919
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([ 5.5793,  8.6449,  8.6271,  8.6107,  8.5985, 11.4784, 11.4660, 11.4518],
       grad_fn=<IndexBackward0>)
tensor([ 1.4091, 45.1660,  6.8944,  1.3910,  0.4434, 45.6640,  8.7781,  1.4091])

        Epoch 0003 | Training loss 24.392866 | Training R2 -0.610849 | Validation loss 31.869343 | Validation R2 -1.480939
        Best loss 29.148003 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.58it/s]
tensor([ 5.8613, 10.4141, 10.1605,  9.9754], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0004 | Training loss 20.007446 | Training R2 -0.083708 | Validation loss 23.670774 | Validation R2 -0.368658
        Best loss 23.670774 | Best epoch 0004

100%|##########################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([10.7725, 17.4414, 16.9693, 15.8382, 21.2687, 19.7636, 24.7900, 23.0800,
        27.9219, 25.9787], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0005 | Training loss 19.205898 | Training R2 0.001384 | Validation loss 22.241131 | Validation R2 -0.208325
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([13.6329, 20.3223, 19.5666, 17.8168, 23.6848, 22.6136, 20.6065, 26.5026,
        25.2495, 23.9893, 22.9034], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])
```

```
        Epoch 0006 | Training loss 20.557449 | Training R2 -0.144109 | Validation loss 24.015671 | Validation R2 -0.488832
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([16.9284, 21.0471, 20.9418, 20.8352, 20.7271, 20.3929, 23.8760, 23.4270,
        22.9282, 26.1789, 25.6684, 25.1570, 28.0688, 27.3257, 30.1612, 29.3570,
        32.1722, 31.3065, 34.1266, 33.1985, 35.9462, 34.9561, 37.6573, 36.6051,
        39.2385, 38.1246, 40.6862, 39.5110, 42.0308, 40.7943],
       grad_fn=<IndexBackward0>)
tensor([38.1730, 32.4920, 24.8420, 20.1090, 16.9610, 11.5390, 42.3870, 24.3350,
        16.9860, 47.3100, 27.9650, 19.6630, 34.2530, 20.9790, 35.0450, 21.5240,
        35.5990, 21.8790, 36.1540, 22.2220, 36.2560, 22.3030, 36.3190, 22.3450,
        36.2250, 22.2940, 36.0400, 22.1840, 35.9840, 22.1450])

        Epoch 0007 | Training loss 20.864714 | Training R2 -0.178566 | Validation loss 24.533953 | Validation R2 -0.470297
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:29<00:00,  7.51it/s]
tensor([13.5987, 17.2932, 17.1564, 17.0169], grad_fn=<IndexBackward0>)
tensor([31.1600, 21.5030, 17.4770, 14.5830])

        Epoch 0008 | Training loss 20.585428 | Training R2 -0.147226 | Validation loss 24.066521 | Validation R2 -0.414805
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 9.4386, 16.3450, 14.2150, 11.4437, 16.6023, 15.0743],
       grad_fn=<IndexBackward0>)
tensor([ 9.5449, 37.6970,  6.5141,  0.8206, 37.8140,  9.5449])

        Epoch 0009 | Training loss 19.902319 | Training R2 -0.072350 | Validation loss 23.161474 | Validation R2 -0.310395
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([ 5.5932, 12.3538, 12.0206, 11.6848, 10.3945,  9.4810,  8.2765,  7.3738],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0010 | Training loss 19.259192 | Training R2 -0.004165 | Validation loss 22.403614 | Validation R2 -0.226044
        Best loss 22.241131 | Best epoch 0005

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 7.3921, 15.4699, 12.9607, 10.8167,  8.3234, 16.6326, 13.7868, 10.9830,
         8.6877, 16.5475, 14.0182, 11.2736,  8.7886, 15.5458, 13.3381, 10.9156,
         8.5450, 13.5284, 12.2548,  9.8752,  7.6965, 12.9978, 10.7930,  8.5555,
         6.4607, 11.1752,  9.0147,  5.6914,  4.6343,  6.9687,  4.7241,  2.6200,
         7.4725,  0.9763,  5.9411,  3.7118, -0.5238,  1.9366,  0.0317, -2.3644,
        -0.0617, -2.3752, -4.5300, -0.0170, -2.3218, -4.7410, -7.4294],
       grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866, 20.7580,  9.6001,  2.4950,  0.7861, 39.1950,  9.6000,  2.4949,
         0.7861, 37.7600,  9.2488,  1.3492,  0.7573,  9.2427,  2.4021,  0.7568,
        42.0710,  0.8422, 45.0040, 11.0200,  0.9023, 11.0300,  3.4749,  0.9031,
        11.0300,  2.8665,  0.9031, 45.0330, 11.0300,  2.8665,  0.7450])

        Epoch 0011 | Training loss 18.370600 | Training R2 0.086359 | Validation loss 20.881422 | Validation R2 -0.065099
        Best loss 20.881422 | Best epoch 0011

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([ 6.5970, 11.4671,  7.1559, 11.7921,  9.5270,  7.0336, 11.2793,  9.2502,
         6.8160, 10.6249,  8.9877,  6.4109, 10.4517,  8.3311,  5.9003,  9.3980,
         5.0892,  8.5680,  6.4435,  3.8118,  7.4316,  5.2236,  2.4744,  6.9502,
         4.0339,  2.3123,  0.8804,  4.4167,  2.0192, -0.9629,  0.0474, -3.0528,
        -1.1970, -3.4509], grad_fn=<IndexBackward0>)
tensor([ 7.5182, 15.6800,  3.1867, 27.9940, 10.3060,  3.4217, 32.5420, 11.7100,
         3.4396, 32.5520, 13.2420,  3.4408, 40.3530, 12.2300,  3.5924, 29.4830,
         3.6040, 32.6680, 11.7570,  3.4535, 34.8010, 12.2340,  3.5934, 34.9970,
        13.8700,  6.6497,  3.6041, 34.1050, 12.2730,  3.6049, 12.2740,  3.6054,
        17.7370,  7.5182])

        Epoch 0012 | Training loss 17.796364 | Training R2 0.142584 | Validation loss 20.198370 | Validation R2 0.003442
        Best loss 20.198370 | Best epoch 0012

100%|##########################################################################| 672/672 [01:29<00:00,  7.55it/s]
tensor([18.1552, 22.1167, 18.2234, 23.1250, 20.6723, 16.5251, 21.2824, 18.8539,
        15.4051, 19.8181, 17.8533, 15.0033, 19.0660, 17.3397, 14.4262, 18.4159],
       grad_fn=<IndexBackward0>)
tensor([46.6430, 16.5660,  2.9642, 47.5600, 16.8100,  3.0078, 47.1240, 16.6500,
         2.9791, 47.5720, 16.8140,  3.0085, 47.0390, 16.6260,  2.9749, 46.6430])

        Epoch 0013 | Training loss 17.672243 | Training R2 0.154502 | Validation loss 20.135670 | Validation R2 0.009620
        Best loss 20.135670 | Best epoch 0013

100%|##########################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([15.7235, 21.9340, 21.4483, 20.9525, 19.3949, 21.5689, 25.2046, 23.9585,
        22.7006, 25.1933, 23.5008, 25.3662, 24.0588, 26.2581, 24.4513, 26.5796,
        24.7060, 27.2621, 24.8573, 26.8676, 25.2804], grad_fn=<IndexBackward0>)
tensor([20.9330, 26.7620, 22.9870, 19.9020, 13.8070, 17.6410, 46.8390, 29.5720,
        19.3340, 35.8980, 20.3400, 31.7000, 20.7250, 36.8060, 20.8550, 36.8910,
        20.9040, 42.8090, 20.9210, 36.9340, 20.9280])

        Epoch 0014 | Training loss 16.964031 | Training R2 0.220911 | Validation loss 19.311337 | Validation R2 0.089050
        Best loss 19.311337 | Best epoch 0014

100%|##########################################################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([17.8863, 37.3666, 32.3489, 23.9999, 39.5029, 35.9349, 28.6494, 38.7055,
        35.1126, 28.4681, 37.0100, 33.2479, 29.0802, 30.2658, 36.5677, 31.0483,
        37.3955, 35.5460, 32.0257, 38.4204, 36.4113, 32.7683],
       grad_fn=<IndexBackward0>)
tensor([ 6.5237, 74.1680, 27.8270,  6.0609, 78.2140, 29.7730,  6.4850, 78.5910,
        29.9390,  6.5212, 78.6230, 29.9530,  6.5243,  6.5245, 63.0610,  6.4075,
        64.1270, 29.9090,  6.5146, 78.6170, 29.9510,  6.5237])

        Epoch 0015 | Training loss 16.071217 | Training R2 0.300759 | Validation loss 18.356150 | Validation R2 0.176937
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([16.5277, 44.4044, 39.2769, 27.7244, 45.6794, 40.7189, 32.3551, 44.8518,
        38.4719, 30.6690], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.0520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.0935])

        Epoch 0016 | Training loss 16.231964 | Training R2 0.286701 | Validation loss 18.394156 | Validation R2 0.173525
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 5.3319, 17.4150, 16.5360, 15.6327, 11.7102,  8.7342,  5.1355,  2.4899],
       grad_fn=<IndexBackward0>)
tensor([ 1.0703, 24.1780, 18.6400, 14.5690,  5.5683,  2.7131,  1.0403,  0.5069])

        Epoch 0017 | Training loss 16.121244 | Training R2 0.296399 | Validation loss 18.390121 | Validation R2 0.173888
        Best loss 18.356150 | Best epoch 0015

100%|##########################################################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([ 8.2026, 28.0302, 26.6790, 23.8754, 20.0850, 16.5093, 11.9295,  8.6301,
         5.4420, 24.6861, 16.0909,  8.5960,  4.5533, 18.9753, 15.0632,  9.7732,
         6.4840], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089])

        Epoch 0018 | Training loss 13.867579 | Training R2 0.479369 | Validation loss 15.791674 | Validation R2 0.390847
        Best loss 15.791674 | Best epoch 0018

100%|##########################################################################| 672/672 [01:37<00:00,  6.91it/s]
tensor([ 6.1014e+00,  2.5528e+01,  1.4262e+01,  5.9708e+00, -2.2717e+00,
         1.6885e+01,  6.1398e+00,  3.2727e-01, -3.4941e+00,  1.1665e+01,
         5.4953e+00,  3.5982e-01, -3.4189e+00,  1.1026e+01,  5.0514e+00,
         7.2515e-04, -3.6842e+00], grad_fn=<IndexBackward0>)
tensor([ 0.7450, 40.8280,  9.9731,  3.1421,  0.8166, 40.8800, 10.0110,  2.6018,
         0.8197, 40.8630, 10.0090,  2.6011,  0.8195, 39.2230,  9.6072,  2.4968,
         0.7866])

        Epoch 0019 | Training loss 12.710710 | Training R2 0.562610 | Validation loss 14.843241 | Validation R2 0.461820
        Best loss 14.843241 | Best epoch 0019

100%|##########################################################################| 672/672 [01:45<00:00,  6.39it/s]
tensor([10.6566, 46.4687, 26.5691, 10.1913,  2.7001, 35.4857, 14.4463,  7.3089,
         1.1632], grad_fn=<IndexBackward0>)
tensor([ 4.6511, 55.9800, 16.9540,  4.6838,  2.0962, 47.9720, 12.9760,  5.8075,
         2.2130])

        Epoch 0020 | Training loss 11.812094 | Training R2 0.622269 | Validation loss 13.195599 | Validation R2 0.574668
        Best loss 13.195599 | Best epoch 0020

100%|##########################################################################| 672/672 [01:59<00:00,  5.64it/s]
tensor([10.1553, 18.2987,  5.9339,  0.7742, 24.4130, 11.2959,  0.2882, 10.9734,
         0.3400, 22.0324,  0.4522,  4.2867,  0.6211, 23.1974,  5.1732,  1.2618,
         0.8361,  8.2529,  1.1520, 23.7739,  4.9145,  1.9538,  1.5326,  9.5868],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.8860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727, 17.5920,
         2.8681, 53.1470,  2.9466,  6.7516,  2.9232, 53.6570,  7.9089,  3.4208,
         2.9753, 11.9150,  2.9524, 53.4760,  6.8475,  3.4086,  2.9648, 14.9510])

        Epoch 0021 | Training loss 10.502948 | Training R2 0.701358 | Validation loss 11.709469 | Validation R2 0.665077
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:23<00:00,  4.69it/s]
tensor([ 4.8642, 17.7674,  3.7490, -0.9090], grad_fn=<IndexBackward0>)
tensor([ 5.8484, 17.8220,  6.0592,  2.8044])

        Epoch 0022 | Training loss 9.577409 | Training R2 0.751672 | Validation loss 12.240973 | Validation R2 0.633983
        Best loss 11.709469 | Best epoch 0021

100%|##########################################################################| 672/672 [02:36<00:00,  4.28it/s]
tensor([10.1105, 54.1474, 47.1999, 40.6521, 34.9629, 18.5855, 10.9887,  5.3792,
         3.3805], grad_fn=<IndexBackward0>)
tensor([12.0510, 55.8980, 40.4280, 31.6660, 25.7020, 12.4280,  7.3585,  3.6646,
```

```
         2.1727])

        Epoch 0023 | Training loss 7.726895 | Training R2 0.838364 | Validation loss 9.112268 | Validation R2 0.797174
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:33<00:00,  4.37it/s]
tensor([ 6.9046, 41.2925, 34.5210, 23.4426, 12.2643,  5.9188,  1.2359, -0.0414,
        -0.5284, 38.4061,  9.3305, -0.1065, -1.4874, 31.3701,  6.5284, -1.4669,
        -2.4291, 13.1051, -1.7246, -3.2997], grad_fn=<IndexBackward0>)
tensor([ 4.8044, 39.7300, 31.8010, 22.1240, 13.5590,  8.3876,  4.4262,  2.7406,
         1.6970, 51.6670, 13.3870,  4.3702,  1.6755, 39.7860, 11.6310,  3.7990,
         1.7089, 18.7290,  4.4247,  1.6964])

        Epoch 0024 | Training loss 9.422968 | Training R2 0.759617 | Validation loss 9.542447 | Validation R2 0.777572
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [02:46<00:00,  4.04it/s]
tensor([23.6239, 67.3576, 30.3424, 17.5867, 53.2716, 29.3855, 18.8101, 57.4894,
        31.0669, 19.9989, 59.8965], grad_fn=<IndexBackward0>)
tensor([42.1750, 56.1960,  7.7854,  0.4302, 32.9930,  7.7374,  0.4275, 41.1230,
         7.5177,  0.4154, 42.1750])

        Epoch 0025 | Training loss 7.962917 | Training R2 0.828338 | Validation loss 9.609860 | Validation R2 0.774418
        Best loss 9.112268 | Best epoch 0023

100%|##########################################################################| 672/672 [03:02<00:00,  3.69it/s]
tensor([  4.8900,  45.6167,   9.5987,   0.1051,  -0.9369,  39.9992,   8.5798,
         -0.3131,  -1.5515,  39.4073,   9.3195,  -0.3392,  -2.4984,  37.1201,
          8.8991,  -0.9208,  -3.5922,  35.8086,   8.4388,  -1.9218,  -4.8642,
         33.2721,   7.2729,  -3.1486,  -6.2217,  31.8621,   6.4087,  -4.3224,
         -7.6073,  29.6215,   4.9850,  -5.7174,  -8.7939,  28.9204,   4.8174,
         -6.7392,  -9.6808,   7.2845,  -6.6397, -10.4594,  26.3305,   1.3159,
         -8.2648, -11.1160,  24.3990,  -0.4301,  -9.1098, -11.8479,  21.2692,
         -2.0180,  -9.9808, -12.4354,  18.3305,  -3.3384, -13.0876,  -4.3371,
        -11.5662, -13.8299,  17.7920, -14.3870,  -4.9450, -12.6202, -15.1504],
       grad_fn=<IndexBackward0>)
tensor([ 1.6133, 40.1610, 12.3810,  4.1701,  1.6409, 41.0410, 12.7110,  4.2813,
         1.6846, 42.8210, 13.2660,  4.4680,  1.7581, 41.6580, 12.9060,  4.3470,
         1.7105, 41.2450, 12.7800,  4.3043,  1.6937, 39.8740, 12.3490,  4.1591,
         1.6366, 39.6830, 12.2880,  4.1388,  1.6285, 38.6890, 11.9880,  4.0377,
         1.5888, 39.3970, 12.2020,  4.1098,  1.6171, 16.2880,  4.6939,  1.5810,
        39.7140, 12.3040,  4.1439,  1.6306, 39.4100, 12.2100,  4.1124,  1.6182,
        37.9910, 11.7700,  3.9642,  1.5598, 36.4990, 11.3100,  1.4989, 11.3470,
         3.8219,  1.5038, 39.1180,  1.6059, 12.1740,  4.1001,  1.6133])

        Epoch 0026 | Training loss 8.169349 | Training R2 0.819323 | Validation loss 8.430163 | Validation R2 0.826403
        Best loss 8.430163 | Best epoch 0026

100%|##########################################################################| 672/672 [03:01<00:00,  3.71it/s]
tensor([ 6.5499, 48.5983, 15.1371,  3.5329], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0027 | Training loss 6.878480 | Training R2 0.871910 | Validation loss 7.949504 | Validation R2 0.845635
        Best loss 7.949504 | Best epoch 0027

100%|##########################################################################| 672/672 [02:57<00:00,  3.79it/s]
tensor([22.4853, 65.2880, 29.7628, 19.7173, 17.9791, 57.3877, 28.7129, 17.0198,
        16.9415, 26.9971, 16.9828, 63.2698, 30.2553, 16.8464, 63.8235, 30.3975,
        16.6662, 63.3403], grad_fn=<IndexBackward0>)
tensor([54.4230, 51.9620, 17.0410,  7.0369,  2.5077, 43.8090, 17.6270,  3.0059,
         2.5940, 15.3480,  2.6174, 55.5800, 18.3240,  2.6966, 55.2450, 18.2160,
         2.6806, 54.4230])

        Epoch 0028 | Training loss 6.115299 | Training R2 0.898757 | Validation loss 5.728622 | Validation R2 0.919838
        Best loss 5.728622 | Best epoch 0028

100%|##########################################################################| 672/672 [02:53<00:00,  3.87it/s]
tensor([ 9.6481, 86.3610, 29.5480,  5.6376, 78.3233, 26.1667,  6.2007, 78.8224,
        24.1587,  6.6242], grad_fn=<IndexBackward0>)
tensor([ 3.5346, 75.5620, 25.2660,  3.8933, 65.0520, 23.0200,  4.0963, 64.9580,
        19.9220,  4.0935])

        Epoch 0029 | Training loss 6.373678 | Training R2 0.890021 | Validation loss 7.142794 | Validation R2 0.875375
        Best loss 5.728622 | Best epoch 0028

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 5 --model 4 --save fold_5 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:27<00:00,  7.65it/s]
tensor([2.4257, 5.2958, 5.4951], grad_fn=<IndexBackward0>)
tensor([16.0320, 54.3750, 13.4380])

        Epoch 0001 | Training loss 25.501337 | Training R2 -0.760577 | Validation loss 32.142315 | Validation R2 -1.523621
        Best loss 32.142315 | Best epoch 0001

100%|##########################################################################| 672/672 [01:27<00:00,  7.68it/s]
tensor([10.9708, 16.4202, 16.4284, 16.4365, 16.4447, 16.4853, 16.5342, 16.5586,
        16.5830, 21.8501, 21.9070, 21.9640, 22.0047], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947])

        Epoch 0002 | Training loss 25.554596 | Training R2 -0.767938 | Validation loss 33.443089 | Validation R2 -1.732012
        Best loss 32.142315 | Best epoch 0001

100%|##########################################################################| 672/672 [01:27<00:00,  7.68it/s]
tensor([ 7.0450, 10.0154, 10.0010,  9.9866], grad_fn=<IndexBackward0>)
tensor([21.4040, 31.6970, 25.8410, 21.4040])

        Epoch 0003 | Training loss 24.312588 | Training R2 -0.600264 | Validation loss 32.068600 | Validation R2 -1.512059
        Best loss 32.068600 | Best epoch 0003

100%|##########################################################################| 672/672 [01:28<00:00,  7.62it/s]
tensor([ 4.0094,  7.7182,  7.1797,  6.7086, 10.2464,  8.3896, 11.8718,  9.6665,
        13.0503, 10.4877, 11.8137, 10.9202, 11.9601], grad_fn=<IndexBackward0>)
tensor([ 2.5158, 10.0050,  2.5792,  0.8070, 40.4740,  0.8047, 40.4720,  0.8047,
        39.6060,  0.7875,  2.5158,  0.7872,  2.5158])

        Epoch 0004 | Training loss 18.267012 | Training R2 0.096633 | Validation loss 19.870958 | Validation R2 0.035488
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:28<00:00,  7.62it/s]
tensor([ 4.8698,  9.7944,  7.7008, 13.1650, 11.7143], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0005 | Training loss 18.761860 | Training R2 0.047026 | Validation loss 21.200550 | Validation R2 -0.097903
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([21.4091, 34.6569, 32.5763], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0006 | Training loss 17.982162 | Training R2 0.124587 | Validation loss 20.414364 | Validation R2 -0.017986
        Best loss 19.870958 | Best epoch 0004

100%|##########################################################################| 672/672 [01:28<00:00,  7.60it/s]
tensor([18.8598, 29.9787, 27.4882], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0007 | Training loss 16.927532 | Training R2 0.224260 | Validation loss 19.159618 | Validation R2 0.103307
        Best loss 19.159618 | Best epoch 0007

100%|##########################################################################| 672/672 [01:28<00:00,  7.60it/s]
tensor([17.9655, 34.3182, 30.5375, 23.3251, 34.3692, 29.5117, 18.7665, 22.5827,
        16.5382, 13.3714, 16.2217, 13.3905, 11.9360, 14.2540, 12.4377, 11.5434,
        13.4844, 12.0562], grad_fn=<IndexBackward0>)
tensor([ 7.2463, 70.3430, 22.7780,  3.3003, 60.2640, 24.0900,  3.4903, 24.0210,
         8.4887,  3.4804, 20.9620,  7.4078,  3.5238, 20.8010,  7.3509,  3.4968,
        20.5050,  7.2463])

        Epoch 0008 | Training loss 16.370752 | Training R2 0.274452 | Validation loss 18.973333 | Validation R2 0.120659
        Best loss 18.973333 | Best epoch 0008

100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([12.1032, 24.9848, 20.8033, 13.0126, 22.6410, 17.7574,  9.1748,  8.4137,
        14.9725, 11.3985,  7.3387, 11.5282,  9.2648,  7.5464, 10.3042,  9.3327,
         7.9984, 10.2717,  9.5589,  8.7520, 10.6169, 10.2095,  9.4622, 11.3097,
        10.8562, 10.0053, 11.4501, 10.8654, 10.3499, 11.8088, 11.2397, 10.5846,
        11.9419, 10.5950, 11.9133, 11.2289, 10.4416, 11.6993, 10.9565, 10.1020,
        11.3339, 10.4162], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9219,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568, 46.7250, 14.1790,  2.9953, 45.9950, 15.9860,
         2.9515, 45.8260, 15.7550,  2.9235, 46.3120, 16.0030,  2.9695, 46.4360,
        16.0330,  2.9750, 20.4610,  7.2470,  2.9262, 21.0770,  8.4980,  3.0144,
        20.5900,  2.9448, 20.6570,  8.3285,  2.9543, 20.5540,  8.2870,  2.9396,
        20.8050,  7.3688])

        Epoch 0009 | Training loss 14.815959 | Training R2 0.405723 | Validation loss 16.785484 | Validation R2 0.311764
        Best loss 16.785484 | Best epoch 0009

100%|##########################################################################| 672/672 [01:28<00:00,  7.56it/s]
tensor([15.2201, 37.9792, 30.4121, 22.7532, 16.1195, 34.4087, 22.6515],
       grad_fn=<IndexBackward0>)
```

```
tensor([15.0620, 56.9590, 15.1310,  4.2726,  1.4454, 56.5590, 15.0620])

        Epoch 0010 | Training loss 14.673149 | Training R2 0.417125 | Validation loss 16.793373 | Validation R2 0.311117
        Best loss 16.785484 | Best epoch 0009

100%|##########################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([12.6484, 24.5527,  9.3701, 16.1193,  8.5453, 18.2315, 13.3730,  8.7617],
       grad_fn=<IndexBackward0>)
tensor([23.5920, 20.2570,  2.7573, 21.0380,  2.8637, 70.1770, 21.0260,  2.8620])

        Epoch 0011 | Training loss 13.782256 | Training R2 0.485755 | Validation loss 15.996996 | Validation R2 0.374904
        Best loss 15.996996 | Best epoch 0011

100%|##########################################################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([ 4.0998, 27.8276, 26.2090, 24.5929, 18.1533, 13.3494,  7.2182,  3.3014,
        21.8690, 13.4942,  8.6837], grad_fn=<IndexBackward0>)
tensor([ 0.4137, 29.3630, 22.5580, 17.5020,  6.4361,  3.0432,  1.1209,  0.2506,
        39.4790,  6.4477,  1.1231])

        Epoch 0012 | Training loss 13.303948 | Training R2 0.520829 | Validation loss 15.555521 | Validation R2 0.408930
        Best loss 15.555521 | Best epoch 0012

100%|##########################################################################| 672/672 [01:29<00:00,  7.47it/s]
tensor([ 9.7279, 32.9579, 31.1551, 27.5726, 20.4980, 15.2696,  8.3477,  2.3601,
        19.6387, 10.3360,  5.2515,  2.0294, 14.1004,  8.3174,  4.3076,  1.9895,
        11.4774,  8.7851,  4.2783,  3.9683, 10.1298,  7.9004,  6.9519,  5.8924,
        11.1614,  9.8574,  8.5018,  7.2632, 12.1099, 10.6080,  9.4548,  8.2704,
        12.6488, 11.3100,  9.9475,  8.7581, 12.8870, 11.5066],
       grad_fn=<IndexBackward0>)
tensor([12.5050, 42.8500, 34.8410, 24.5230, 12.4040,  7.4428,  3.7669,  1.3563,
        42.1990, 12.2480,  3.7197,  1.3393, 42.1710, 12.2410,  3.7175,  1.3385,
        43.0630, 20.8330,  1.9210,  1.3667, 43.0860,  8.8969,  3.7979,  1.3674,
        42.5380, 12.3470,  3.7496,  1.3500, 42.9850, 10.5230,  3.7888,  1.3642,
        43.0840, 12.5050,  3.7977,  1.3674, 43.0840, 12.5050])

        Epoch 0013 | Training loss 13.012312 | Training R2 0.541607 | Validation loss 15.213802 | Validation R2 0.434613
        Best loss 15.213802 | Best epoch 0013

100%|##########################################################################| 672/672 [01:29<00:00,  7.48it/s]
tensor([ 0.2745, 10.0347,  2.2603, -0.2056, -0.6719,  8.2394,  3.7114,  1.4496,
         1.0090,  8.3221,  4.2308,  2.6189,  2.3726,  7.1274,  5.6220,  4.6618,
         4.4669,  8.3041,  7.0924,  5.9960,  5.8123,  9.2877,  7.8543,  6.7494,
        10.1614,  8.6661,  7.3556, 10.6087,  8.6601,  7.7160, 10.9884,  9.1611,
         7.9981, 11.2231,  9.1500,  8.1591, 11.2712,  9.3742],
       grad_fn=<IndexBackward0>)
tensor([ 5.3298, 14.0900,  5.0763,  2.4483,  2.1161, 14.7070,  5.2983,  2.5554,
         2.2086, 14.9430,  5.3834,  2.5964,  2.2441, 12.6780,  5.2850,  2.5490,
         2.2031, 16.6050,  5.9815,  2.4934,  2.1551, 16.9430,  5.2750,  2.1989,
        19.6280,  6.1089,  2.2010, 19.5260,  4.5398,  2.1895, 19.9330,  5.3619,
         2.2351, 20.0550,  4.6626,  2.2488, 19.8140,  5.3298])

        Epoch 0014 | Training loss 12.533939 | Training R2 0.574691 | Validation loss 14.716722 | Validation R2 0.470956
        Best loss 14.716722 | Best epoch 0014

100%|##########################################################################| 672/672 [01:30<00:00,  7.44it/s]
tensor([ 6.7641, 18.5638,  6.5979, 23.9049, 15.6916], grad_fn=<IndexBackward0>)
tensor([12.8470, 12.6880,  1.0025, 53.5960, 12.8470])

        Epoch 0015 | Training loss 12.104251 | Training R2 0.603352 | Validation loss 14.334991 | Validation R2 0.498045
        Best loss 14.334991 | Best epoch 0015

100%|##########################################################################| 672/672 [01:30<00:00,  7.40it/s]
tensor([13.9795, 46.5063, 19.0063,  4.8340, 29.5911, 16.0146,  4.8011, 21.8338,
        12.8681,  4.3595], grad_fn=<IndexBackward0>)
tensor([14.0340, 52.5400, 13.3690,  1.8996, 54.8650, 14.0150,  1.9913, 37.1760,
        11.8580,  1.9824])

        Epoch 0016 | Training loss 11.550217 | Training R2 0.638832 | Validation loss 13.747127 | Validation R2 0.538370
        Best loss 13.747127 | Best epoch 0016

100%|##########################################################################| 672/672 [01:31<00:00,  7.34it/s]
tensor([ 4.0921, 18.3844,  3.6786, 16.8184,  5.1207, 14.0996,  5.4195, 14.2547,
         6.1746, 13.5347,  6.7133, 14.0622, 10.0545,  7.3826, 10.5945,  8.0517,
        11.2127,  8.8817, 15.2608, 11.8977,  9.8144, 12.7852, 10.7657, 13.3178,
        11.8928, 11.6402, 14.6168, 12.6066, 15.4988, 13.4973],
       grad_fn=<IndexBackward0>)
tensor([ 2.9329, 18.1390,  2.8114, 19.1060,  2.9618, 16.6620,  2.9542, 19.3020,
         2.9922, 19.2630,  2.9861, 19.0680,  7.4988,  2.9560,  7.4813,  2.9491,
         7.4269,  2.9277, 19.0190,  7.4794,  2.9484,  7.5152,  2.9625,  6.4918,
         3.3388,  2.9231,  7.5188,  2.9639,  7.4401,  2.9329])

        Epoch 0017 | Training loss 11.089778 | Training R2 0.667053 | Validation loss 13.340640 | Validation R2 0.565266
        Best loss 13.340640 | Best epoch 0017

100%|##########################################################################| 672/672 [01:32<00:00,  7.29it/s]
tensor([16.4245, 59.1090, 21.8380], grad_fn=<IndexBackward0>)
tensor([13.8520, 68.8710, 23.1830])

        Epoch 0018 | Training loss 10.320528 | Training R2 0.711641 | Validation loss 11.873363 | Validation R2 0.655636
        Best loss 11.873363 | Best epoch 0018

100%|##########################################################################| 672/672 [01:33<00:00,  7.19it/s]
tensor([17.6073, 63.8990, 24.1658,  5.6614, 44.2576, 22.5470,  6.5664],
       grad_fn=<IndexBackward0>)
tensor([17.6690, 69.9310, 19.6240,  2.0229, 70.4890, 19.8330,  2.0444])

        Epoch 0019 | Training loss 9.479305 | Training R2 0.756734 | Validation loss 11.307576 | Validation R2 0.687673
        Best loss 11.307576 | Best epoch 0019

100%|##########################################################################| 672/672 [01:35<00:00,  7.03it/s]
tensor([22.7205, 66.0948, 26.8823, 15.5828], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0020 | Training loss 8.340364 | Training R2 0.811679 | Validation loss 8.864890 | Validation R2 0.808037
        Best loss 8.864890 | Best epoch 0020

100%|##########################################################################| 672/672 [01:39<00:00,  6.74it/s]
tensor([10.0821, 26.9367, 20.8400, 17.0122, 11.5361, 15.8813, 36.3308, 25.5300,
        17.7422, 30.3660, 18.7054, 27.2397, 19.3506, 30.3209, 19.6491],
       grad_fn=<IndexBackward0>)
tensor([20.9330, 26.7620, 22.9870, 19.9020, 13.0070, 17.6410, 46.8390, 29.5720,
        19.3340, 35.8980, 20.3400, 31.7000, 20.7250, 36.8060, 20.8550])

        Epoch 0021 | Training loss 7.650942 | Training R2 0.841526 | Validation loss 8.756156 | Validation R2 0.812718
        Best loss 8.756156 | Best epoch 0021

100%|##########################################################################| 672/672 [01:45<00:00,  6.39it/s]
tensor([ 3.7506, 33.9919,  8.2549,  1.2967, -1.8662, -2.1911, 12.2417,  1.5280,
        -1.5885, -1.8975, 11.5778,  2.3445, -1.2041, -1.4682],
       grad_fn=<IndexBackward0>)
tensor([ 0.4168, 38.0910,  7.1683,  1.7787,  0.4414,  0.3499, 11.5080,  1.7944,
         0.4453,  0.3530, 10.8300,  2.1303,  0.4190,  0.3322])

        Epoch 0022 | Training loss 6.915258 | Training R2 0.870537 | Validation loss 6.888650 | Validation R2 0.884085
        Best loss 6.888650 | Best epoch 0022

100%|##########################################################################| 672/672 [01:57<00:00,  5.71it/s]
tensor([ 1.5398,  4.4927,  3.3403,  2.5443,  1.9098,  0.1433, -0.4094, -0.6202,
        -0.6513, -0.6544,  2.8599, -0.0619, -0.3231, -0.5211, -0.5408,  2.8718,
         0.0123, -0.4279, -0.4479], grad_fn=<IndexBackward0>)
tensor([0.1027, 4.3675, 3.3207, 2.6789, 2.2198, 1.1160, 0.6726, 0.3426, 0.2066,
        0.1245, 4.4427, 1.1442, 0.8164, 0.3513, 0.1277, 4.4458, 1.1451, 0.3516,
        0.1278])

        Epoch 0023 | Training loss 6.409317 | Training R2 0.888788 | Validation loss 6.464874 | Validation R2 0.897908
        Best loss 6.464874 | Best epoch 0023

100%|##########################################################################| 672/672 [02:15<00:00,  4.94it/s]
tensor([ 9.2943, 67.5948, 20.8247,  3.1299, 21.1432,  4.3623, 20.8246,  4.6365,
        21.1392,  5.1836], grad_fn=<IndexBackward0>)
tensor([ 2.0389, 55.6560, 16.1950,  2.1895, 15.9180,  2.1521, 15.2060,  2.0559,
        15.0810,  2.0389])

        Epoch 0024 | Training loss 6.434866 | Training R2 0.887899 | Validation loss 6.995244 | Validation R2 0.880470
        Best loss 6.464874 | Best epoch 0023

100%|##########################################################################| 672/672 [02:24<00:00,  4.66it/s]
tensor([ 7.0800, 75.9345, 57.3135, 47.6548, 39.5218, 14.2651,  2.0937, -0.6384,
        -2.3179, 56.9519, 15.1308,  2.2615, -1.0054, 57.1468, 16.1390,  3.2208,
         0.1911], grad_fn=<IndexBackward0>)
tensor([ 1.7195, 93.2850, 73.9670, 62.0350, 53.2360, 26.3850, 11.4810,  7.5733,
         4.9958, 75.1950, 26.9070, 10.1920,  5.0947, 73.8930, 26.4440, 10.0160,
         5.0069])

        Epoch 0025 | Training loss 6.013347 | Training R2 0.902105 | Validation loss 6.196391 | Validation R2 0.906212
        Best loss 6.196391 | Best epoch 0025

100%|##########################################################################| 672/672 [02:27<00:00,  4.54it/s]
tensor([24.2445, 61.1039], grad_fn=<IndexBackward0>)
tensor([47.8150, 46.0380])

        Epoch 0026 | Training loss 6.441009 | Training R2 0.887685 | Validation loss 5.943230 | Validation R2 0.913719
        Best loss 5.943230 | Best epoch 0026

100%|##########################################################################| 672/672 [02:34<00:00,  4.35it/s]
tensor([20.4664, 65.3887, 21.7751], grad_fn=<IndexBackward0>)
tensor([28.6530, 67.5770, 24.1020])

        Epoch 0027 | Training loss 6.147571 | Training R2 0.897686 | Validation loss 5.676152 | Validation R2 0.921299
        Best loss 5.676152 | Best epoch 0027

100%|##########################################################################| 672/672 [02:32<00:00,  4.40it/s]
tensor([ 5.5889, 51.8624, 13.1392,  2.6198], grad_fn=<IndexBackward0>)
tensor([ 1.6420, 52.0970,  9.8003,  1.9523])

        Epoch 0028 | Training loss 6.355262 | Training R2 0.890656 | Validation loss 5.838716 | Validation R2 0.916727
        Best loss 5.676152 | Best epoch 0027

100%|##########################################################################| 672/672 [02:34<00:00,  4.36it/s]
```

```
tensor([10.5076, 63.3576, 17.9138,  3.0357, 61.1687, 18.1363,  3.4611, 61.1664,
        17.9986,  5.9321,  3.2432], grad_fn=<IndexBackward0>)
tensor([ 7.3120, 60.1970, 18.1710,  3.1501, 62.0600, 19.0200,  3.2978, 62.7360,
        19.2460,  7.4859,  3.3370])

        Epoch 0029 | Training loss 6.041739 | Training R2 0.901178 | Validation loss 5.606994 | Validation R2 0.923206
        Best loss 5.606994 | Best epoch 0029

/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:36: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.1
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:40: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.2
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/data_split.py:44: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df["PTNM"] = df["PTNM"] + 0.3
/Users/rishabhgoel/Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py
Desktop/NeuralODE_Paper_Supplementary_Code/5fold_models/Neural-ODE/run_train.py --fold 5 --model 5 --save fold_5 --lr 0.00005 --tol 1e-4 --epochs 30 --l2 0.1
100%|##########################################################################| 672/672 [01:28<00:00,  7.57it/s]
tensor([2.4484, 4.2480, 4.2779, 4.3673, 5.9840, 6.0726, 6.1612, 7.7987, 7.8873,
        7.9464, 9.5586], grad_fn=<IndexBackward0>)
tensor([46.2230, 25.8570, 22.3620, 14.7790, 49.8490, 30.4130, 20.1220, 45.1010,
        29.2020, 22.1960, 46.2230])

        Epoch 0001 | Training loss 25.574455 | Training R2 -0.770688 | Validation loss 32.248924 | Validation R2 -1.540390
        Best loss 32.248924 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 6.8719, 11.2345, 11.2490, 11.2636, 11.3365, 11.3802, 11.4385, 11.5260,
        15.8160, 15.9035, 16.0055, 16.1075, 20.4351, 20.5371, 20.6391],
       grad_fn=<IndexBackward0>)
tensor([ 4.2877, 59.4320, 46.9050, 38.1280, 14.2580,  7.9220,  3.6186,  1.1171,
        59.4890, 17.3990,  4.4157,  1.1207, 17.1950,  4.3640,  1.1075])

        Epoch 0002 | Training loss 25.707258 | Training R2 -0.789125 | Validation loss 33.621529 | Validation R2 -1.761244
        Best loss 32.248924 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([ 8.7414, 12.7972, 12.7764, 12.7377, 16.7811, 16.7605, 16.7220, 20.7506,
        20.7300, 20.6916, 24.7062, 24.6826, 24.6471], grad_fn=<IndexBackward0>)
tensor([22.8850, 73.4140, 23.4880,  3.5482, 76.4500, 24.6180,  3.7189, 76.3100,
        24.5840,  3.7138, 76.0510, 21.1850,  3.7013])

        Epoch 0003 | Training loss 24.666088 | Training R2 -0.647137 | Validation loss 32.497631 | Validation R2 -1.579724
        Best loss 32.248924 | Best epoch 0001

100%|##########################################################################| 672/672 [01:28<00:00,  7.61it/s]
tensor([10.6754, 14.8498, 14.5839, 14.0860, 18.2218, 17.9692, 17.4180, 21.2452,
        20.9197, 20.6395, 24.4369, 24.0812, 23.8262, 27.5497, 27.1639, 26.8873,
        30.5101, 30.0944], grad_fn=<IndexBackward0>)
tensor([ 7.2463, 70.3430, 22.7780,  3.3003, 60.2640, 24.0900,  3.4903, 24.0210,
         8.4887,  3.4804, 20.9620,  7.4078,  3.5238, 20.8010,  7.3509,  3.4968,
        20.5050,  7.2463])

        Epoch 0004 | Training loss 20.829603 | Training R2 -0.174603 | Validation loss 25.828514 | Validation R2 -0.629554
        Best loss 25.828514 | Best epoch 0004

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([16.2147, 21.5864, 21.4826, 21.3787, 21.2745, 20.9608, 26.1750, 25.9152,
        25.3930, 30.5795, 30.1107, 29.6397, 33.4538, 38.3805, 37.3363, 41.9564,
        40.7835, 45.0146, 43.9732, 48.4566, 47.3058, 51.7068, 50.4458, 54.3377,
        52.9737, 56.7880, 55.3201, 59.0563, 57.4837], grad_fn=<IndexBackward0>)
tensor([20.7140, 46.6930, 36.3750, 29.6610, 24.7630, 15.1220, 59.5840, 39.0430,
        20.0970, 63.5550, 35.3180, 21.6870, 21.4910, 52.0110, 22.1980, 50.6250,
        21.6590, 41.1430, 21.2610, 42.8590, 22.1220, 43.3930, 22.4050, 41.0620,
        21.2290, 40.3330, 20.8420, 40.0930, 20.7140])

        Epoch 0005 | Training loss 17.920830 | Training R2 0.130549 | Validation loss 19.372255 | Validation R2 0.083293
        Best loss 19.372255 | Best epoch 0005

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([12.9280, 20.2518, 19.2812, 18.1340], grad_fn=<IndexBackward0>)
tensor([ 2.7552, 54.7350, 20.0870,  7.1519])

        Epoch 0006 | Training loss 17.330109 | Training R2 0.186923 | Validation loss 18.413456 | Validation R2 0.171790
        Best loss 18.413456 | Best epoch 0006

100%|##########################################################################| 672/672 [01:28<00:00,  7.55it/s]
tensor([20.7437, 34.6813, 34.4258, 34.1697, 33.6561, 32.8820, 32.1033, 31.8576,
        30.2675], grad_fn=<IndexBackward0>)
tensor([10.7920, 67.0230, 50.2480, 40.4590, 28.8060, 18.4230, 11.9080,  6.6646,
         4.3127])

        Epoch 0007 | Training loss 16.879265 | Training R2 0.228677 | Validation loss 18.103533 | Validation R2 0.199435
        Best loss 18.103533 | Best epoch 0007

100%|##########################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([13.7128, 30.2793, 27.5493, 22.4059, 31.3710, 27.1914, 21.9170, 20.8554,
        24.8973, 16.4144], grad_fn=<IndexBackward0>)
tensor([ 2.0712, 67.0250, 19.0148,  2.0747, 60.3840, 14.5370,  2.6447,  1.8809,
        16.9540,  1.8498])

        Epoch 0008 | Training loss 16.286880 | Training R2 0.281867 | Validation loss 17.865025 | Validation R2 0.220390
        Best loss 17.865025 | Best epoch 0008

100%|##########################################################################| 672/672 [01:29<00:00,  7.54it/s]
tensor([ 8.4889, 23.1581, 19.7200, 16.2299], grad_fn=<IndexBackward0>)
tensor([ 3.1494, 45.2250, 11.2840,  2.9028])

        Epoch 0009 | Training loss 15.591856 | Training R2 0.341850 | Validation loss 17.282658 | Validation R2 0.270390
        Best loss 17.282658 | Best epoch 0009

100%|##########################################################################| 672/672 [01:29<00:00,  7.52it/s]
tensor([ 0.9627,  7.5878,  7.0483,  6.5082,  3.8039,  2.1405,  0.2473, -0.6598,
        -1.2493,  3.6337,  1.8889,  1.0659,  0.5348,  3.1808,  2.5651,  2.0258,
         1.6292], grad_fn=<IndexBackward0>)
tensor([ 0.2632, 13.4210,  9.5364,  7.0612,  1.7695,  0.7790,  0.2609,  0.1149,
         0.0506, 13.0570,  1.7257,  0.2544,  0.0493, 13.2040,  1.7452,  0.2573,
         0.0499])

        Epoch 0010 | Training loss 14.974828 | Training R2 0.392910 | Validation loss 16.909748 | Validation R2 0.301536
        Best loss 16.909748 | Best epoch 0010

100%|##########################################################################| 672/672 [01:29<00:00,  7.50it/s]
tensor([12.9711, 42.1341, 35.1787, 19.0216, 31.2690, 15.0380, 21.2784, 13.9399],
       grad_fn=<IndexBackward0>)
tensor([ 1.5969, 68.9360, 20.1160,  1.3031, 20.2650,  1.3127, 20.2740,  1.5969])

        Epoch 0011 | Training loss 14.465054 | Training R2 0.433540 | Validation loss 16.548763 | Validation R2 0.331039
        Best loss 16.548763 | Best epoch 0011

100%|##########################################################################| 672/672 [01:30<00:00,  7.45it/s]
tensor([ 0.0758,  2.3892,  1.6755,  0.9163, -0.4983, -1.7617, -2.4187, -2.9047,
        -3.1434], grad_fn=<IndexBackward0>)
tensor([0.0492, 5.6725, 4.1326, 3.1690, 1.9529, 0.9650, 0.4778, 0.1872, 0.0927])

        Epoch 0012 | Training loss 13.845372 | Training R2 0.481035 | Validation loss 15.948896 | Validation R2 0.378657
        Best loss 15.948896 | Best epoch 0012

100%|##########################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([ 9.3530, 21.3644, 11.0038,  7.0158, 20.8011, 13.9052,  7.4559, 11.5265,
         7.7576, 13.3328,  8.3271,  9.8427,  9.4540, 12.3438, 11.0543, 10.6271,
        10.5572, 12.2739, 11.4969, 14.0482, 12.8231, 12.4112, 12.3301, 13.7474],
       grad_fn=<IndexBackward0>)
tensor([14.9510, 17.0860,  6.4340,  2.7857, 51.9570, 17.6200,  2.8727, 17.5920,
         2.8681, 53.1470,  2.9466,  6.7516,  2.9232, 53.6570,  7.9089,  3.4208,
         2.9753, 11.9150,  2.9524, 53.4760,  6.8475,  3.4086,  2.9648, 14.9510])

        Epoch 0013 | Training loss 13.343873 | Training R2 0.517949 | Validation loss 15.788548 | Validation R2 0.391088
        Best loss 15.788548 | Best epoch 0013

100%|##########################################################################| 672/672 [01:30<00:00,  7.41it/s]
tensor([ 6.1348, 15.3637,  4.9847, 16.9890, 10.8584,  5.5472, 13.0540,  9.6103,
         6.1307, 11.4658,  9.0124,  7.1509], grad_fn=<IndexBackward0>)
tensor([ 9.8032,  9.6259,  0.6383, 43.8570,  9.7042,  0.6435, 44.0790,  9.7534,
         0.6467, 44.4320,  9.8362,  0.6522])

        Epoch 0014 | Training loss 12.861094 | Training R2 0.552199 | Validation loss 15.118623 | Validation R2 0.441666
        Best loss 15.118623 | Best epoch 0014

100%|##########################################################################| 672/672 [01:30<00:00,  7.39it/s]
tensor([10.6163, 26.8854, 24.9820, 23.1042, 21.2513, 15.8637, 27.8975, 22.9511,
        17.0839, 28.4169, 18.7819, 26.8114, 19.3796, 26.7333, 18.6195, 25.7249,
        17.9570], grad_fn=<IndexBackward0>)
tensor([21.3340, 19.2610, 14.4950, 11.2260,  8.9585,  5.3881, 18.6970, 12.5000,
         8.2546, 26.5910, 10.1260, 28.1980, 11.3250, 29.3320, 12.1280, 30.0900,
        12.6640])

        Epoch 0015 | Training loss 12.244040 | Training R2 0.594138 | Validation loss 14.156057 | Validation R2 0.510498
        Best loss 14.156057 | Best epoch 0015

100%|##########################################################################| 672/672 [01:31<00:00,  7.33it/s]
tensor([12.8128, 47.7913, 21.1960,  3.6788, 30.4371, 17.4128,  3.3207, 26.1706,
        14.8149,  3.9932, 22.5698, 15.0680,  5.3215,  4.8011, 16.4523,  6.9937,
         6.0652,  8.5227,  7.5822, 17.7124,  9.9428,  9.0986, 19.0299, 11.2369,
        21.8405, 18.8739, 13.2249, 22.8238, 20.1484, 14.9844, 24.0042, 21.8666,
        16.8832, 25.3697, 23.4747, 18.6334, 25.8639, 23.3855, 20.2469, 27.4377,
        25.0003, 21.9271, 28.9922, 23.5628, 27.8851], grad_fn=<IndexBackward0>)
tensor([ 9.0468, 54.6540, 20.0790,  3.7909, 57.0780, 21.1030,  3.9842, 56.9820,
```

```
        21.1180,  3.9872, 57.0060, 21.1240,  4.5338,  3.9882, 27.3110,  5.1542,
         3.9883,  5.1542,  3.9883, 31.0680,  5.1532,  3.9875, 32.2750,  4.1424,
        59.3510, 21.9960,  4.1529, 58.5410, 21.6980,  4.0967, 60.0390, 22.2480,
         4.2004, 59.9030, 22.2010,  4.1916, 32.2840, 13.1400,  4.1436, 32.6290,
        13.2800,  4.1878, 32.6930,  4.1960,  9.0468])

        Epoch 0016 | Training loss 12.546910 | Training R2 0.573810 | Validation loss 16.446472 | Validation R2 0.339283
        Best loss 14.156057 | Best epoch 0015

100%|##########################################################################| 672/672 [01:32<00:00,  7.26it/s]
tensor([25.2400, 63.0524, 30.0123, 18.4202], grad_fn=<IndexBackward0>)
tensor([48.1440, 50.7900,  7.5206,  1.1606])

        Epoch 0017 | Training loss 11.841760 | Training R2 0.620369 | Validation loss 13.399882 | Validation R2 0.561397
        Best loss 13.399882 | Best epoch 0017

100%|##########################################################################| 672/672 [01:33<00:00,  7.17it/s]
tensor([ 3.7582, 17.1202,  2.3787, 24.3760, 13.3095,  2.2700, 17.5527,  9.0142,
         1.3517, 14.9198,  8.1555,  1.1716,  7.7569,  1.2899,  1.5562,  7.3537,
         1.8437, 13.5366,  7.3543,  2.0825,  8.0452,  2.6267,  2.3807,  8.1799,
         2.7442,  3.1212, 13.1283,  8.7356,  3.4417], grad_fn=<IndexBackward0>)
tensor([ 1.7265, 18.3160,  2.4943, 49.3870, 15.7180,  2.1405, 40.9940, 12.9500,
         1.7635, 40.5030, 12.8680,  1.7524, 12.6860,  1.7275,  1.7280, 12.6780,
         1.7266, 39.8550, 12.6780,  1.7265, 14.7770,  2.0123,  1.7262, 14.7770,
         1.7262,  1.7262, 39.8540, 14.7800,  1.7265])

        Epoch 0018 | Training loss 9.960876 | Training R2 0.731389 | Validation loss 11.356238 | Validation R2 0.684979
        Best loss 11.356238 | Best epoch 0018

100%|##########################################################################| 672/672 [01:35<00:00,  7.03it/s]
tensor([ 3.6073, 21.7651,  2.6404,  1.7438, 22.0736,  2.8508, 19.3228,  3.0228],
       grad_fn=<IndexBackward0>)
tensor([ 3.7309, 20.7410,  4.1518,  3.6310, 21.9260,  3.8384, 21.3500,  3.7377])

        Epoch 0019 | Training loss 9.017970 | Training R2 0.779836 | Validation loss 10.003691 | Validation R2 0.755550
        Best loss 10.003691 | Best epoch 0019

100%|##########################################################################| 672/672 [01:38<00:00,  6.80it/s]
tensor([ 3.9709, 21.9546,  2.3444, 18.1305,  3.7273], grad_fn=<IndexBackward0>)
tensor([ 1.9136, 20.0690,  1.9223, 15.1660,  1.9866])

        Epoch 0020 | Training loss 8.921117 | Training R2 0.784540 | Validation loss 10.963613 | Validation R2 0.706386
        Best loss 10.003691 | Best epoch 0019

100%|##########################################################################| 672/672 [01:44<00:00,  6.44it/s]
tensor([ 6.2324, 42.5617, 34.4039, 30.1860, 17.3074, 10.6958,  4.7618,  1.7787,
        -0.3446, 44.9082, 17.6935,  5.0156], grad_fn=<IndexBackward0>)
tensor([ 2.8854, 42.8980, 34.5060, 27.9840, 12.2340,  6.5823,  2.8806,  1.5499,
         0.8339, 54.9410, 12.2540,  2.8854])

        Epoch 0021 | Training loss 7.610228 | Training R2 0.843208 | Validation loss 7.832873 | Validation R2 0.850131
        Best loss 7.832873 | Best epoch 0021

100%|##########################################################################| 672/672 [01:57<00:00,  5.72it/s]
tensor([ 0.8088, 12.1520,  1.4148, -1.9840], grad_fn=<IndexBackward0>)
tensor([ 1.4236, 14.5010,  4.3771,  1.8603])

        Epoch 0022 | Training loss 6.943378 | Training R2 0.869482 | Validation loss 7.526657 | Validation R2 0.861620
        Best loss 7.526657 | Best epoch 0022

100%|##########################################################################| 672/672 [02:13<00:00,  5.05it/s]
tensor([ 9.7984, 18.7175,  7.9693,  4.5303, 43.3811, 19.0467, 13.2996,  8.7738,
         5.3788, 19.4652,  9.1786,  5.8376], grad_fn=<IndexBackward0>)
tensor([17.2550, 16.6050,  5.5696,  2.1836, 53.8670, 17.2450, 10.7980,  5.7840,
         2.2677, 17.4680,  5.8590,  2.2971])

        Epoch 0023 | Training loss 6.863361 | Training R2 0.872473 | Validation loss 7.845010 | Validation R2 0.849666
        Best loss 7.526657 | Best epoch 0022

100%|##########################################################################| 672/672 [02:20<00:00,  4.78it/s]
tensor([13.9296, 50.0027, 14.2701], grad_fn=<IndexBackward0>)
tensor([18.2960, 46.2360, 13.6630])

        Epoch 0024 | Training loss 6.259858 | Training R2 0.893914 | Validation loss 6.466238 | Validation R2 0.897865
        Best loss 6.466238 | Best epoch 0024

100%|##########################################################################| 672/672 [02:25<00:00,  4.61it/s]
tensor([ 5.8438, 19.6714, 16.3584, 13.6462,  7.7119, 27.7933, 16.9801,  9.8968,
        28.9267, 17.5417, 10.3755, 10.5065, 10.6070, 12.6879],
       grad_fn=<IndexBackward0>)
tensor([ 9.5916, 17.5620, 13.7300, 11.0450,  6.0491, 28.0840, 13.4860,  7.4104,
        28.4930, 13.8100,  7.5943,  7.6922,  7.8397,  9.5916])

        Epoch 0025 | Training loss 6.173162 | Training R2 0.896832 | Validation loss 5.846045 | Validation R2 0.916518
        Best loss 5.846045 | Best epoch 0025

100%|##########################################################################| 672/672 [02:28<00:00,  4.53it/s]
tensor([26.9313, 68.0550, 27.3174, 17.6764, 14.2293, 52.9944, 27.5906, 14.8336,
        14.7004, 25.4410, 14.8944, 62.6680, 28.1108, 14.8701, 62.9070, 27.7113,
        14.6878, 62.0197], grad_fn=<IndexBackward0>)
tensor([54.4230, 51.9620, 17.0410,  7.0369,  2.5077, 43.8090, 17.6270,  3.0059,
         2.5940, 15.3480,  2.6174, 55.5800, 18.3240,  2.6966, 55.2450, 18.2160,
         2.6806, 54.4230])

        Epoch 0026 | Training loss 6.230823 | Training R2 0.894896 | Validation loss 5.759395 | Validation R2 0.918974
        Best loss 5.759395 | Best epoch 0026

100%|##########################################################################| 672/672 [02:31<00:00,  4.45it/s]
tensor([ 8.7405, 41.4062, 11.0105,  1.9193, 37.8420, 13.6592,  2.8849,  2.7431,
        37.8419, 13.8848,  3.0083], grad_fn=<IndexBackward0>)
tensor([ 7.3688, 43.7320, 14.9210,  2.7685, 45.9550, 18.0700,  3.8155,  2.9446,
        46.1300, 18.1450,  2.9568])

        Epoch 0027 | Training loss 5.820685 | Training R2 0.908277 | Validation loss 5.586363 | Validation R2 0.923770
        Best loss 5.586363 | Best epoch 0027

100%|##########################################################################| 672/672 [02:31<00:00,  4.44it/s]
tensor([10.6622, 58.6032, 45.5674, 38.3795, 32.1584, 18.5847, 66.5827, 48.5411,
        23.8967, 70.6964, 43.0946, 25.1775, 24.7224, 61.8428, 25.5096, 59.9630,
        24.7325], grad_fn=<IndexBackward0>)
tensor([20.7140, 46.6930, 36.3750, 29.6610, 24.7630, 15.1220, 59.5840, 39.0430,
        20.0970, 63.5550, 35.3180, 21.6870, 21.4910, 52.0110, 22.1980, 50.6250,
        21.6590])

        Epoch 0028 | Training loss 5.790850 | Training R2 0.909215 | Validation loss 5.422966 | Validation R2 0.928164
        Best loss 5.422966 | Best epoch 0028

100%|##########################################################################| 672/672 [02:32<00:00,  4.40it/s]
tensor([17.9213, 91.8541, 30.2644], grad_fn=<IndexBackward0>)
tensor([19.2920, 85.6310, 19.2920])

        Epoch 0029 | Training loss 5.716786 | Training R2 0.911522 | Validation loss 5.752234 | Validation R2 0.919176
        Best loss 5.422966 | Best epoch 0028

(base) rishabhgoel@GEn1Es-MacBook-Pro ~ % PNover
```