**TABLE 1** Hyperparameter space for DNNs.

| Hyperparameter | Values |
|---|---|
| # nodes for first hidden layer | 30, 40, 50, 75, 100, 120, 150 |
| # hidden layers | 4, 5, 6, 8, 10, 15 |
| batch size | 8, 16, 32, 64, 128 |
| activation function | ReLu, sigmoid, tanh, SELU, ELU |
| optimizer | SGD, RMSprop, Adam, Adadelta, Adagrad, Adamax, Nadam, Ftrl |
| learning rate | $10^{-5}$, $10^{-4}$, $10^{-3}$, $10^{-2}$ |
| # epochs | 100, 300, 400, 600, 1000, 1500 |
| preprocessing method | StandartScaler, MinMaxScaler |
| regularization function | None, L2, L1, Dropout |
| regularization rate | $10^{-5}$, $10^{-4}$, $10^{-3}$, $10^{-2}$ |
| dropout rate | 0.2, 0.3, 0.4, 0.5 |
| weight initializer | Xavier Normal or Uniform, He Normal or Uniform, Random Normal or Uniform, Ones |

**TABLE 2** Chosen hyperparameter combinations.

| Hyperparameter | $DNN_{FeFeB}$ | $DNN_{FeFeB-Fe}$ |
|---|---|---|
| # nodes for hidden layers | 120, 108, 96, 84, 72, 60 | 100, 100, 100, 100 |
| batch size | 32 | 32 |
| activation function | ReLu | ELU |
| optimizer | Adamax | Adamax |
| learning rate | $10^{-3}$ | $10^{-3}$ |
| # epochs | 400 | 1500 |
| preprocessing method | StandartScaler | StandartScaler |
| regularization function | None | None |
| weight initializer | Xavier Normal | Xavier Normal |

**TABLE 3** Results of 10–fold cross–validation

| Dataset | MSRE | |
|---|---|---|
| | $\mathbf{DNN}_{FeFeB}$ | $\mathbf{DNN}_{FeFeB-Fe}$ |
| training | 0.31 ± 0.07 | 0.03 ± 0.01 |
| full | 0.28 ± 0.05 | 0.03 ± 0.01 |

**TABLE 4** DNN's testing results

| Dataset | $DNN_{FeFeB}$ | | | $DNN_{FeFeB-Fe}$ | | |
|---|---|---|---|---|---|---|
| | **MSRE** | $R^2$ | $R$ | **MSRE** | $R^2$ | $R$ |
| T–varied | 0.41 | 0.936 | 0.967 | 0.020 | 0.994 | 0.997 |
| d–varied | 0.37 | 0.961 | 0.980 | 0.018 | 0.996 | 0.998 |
| B–varied | 1.06 | 0.881 | 0.939 | 0.084 | 0.991 | 0.995 |
| Fe–varied | 0.06 | 0.991 | 0.996 | 0.005 | 0.999 | 0.999 |
| All–varied | 0.54 | 0.813 | 0.901 | 0.138 | 0.948 | 0.974 |

**TABLE 5** Results of experimental IV fitting and iron contamination testing

| Sample | $N_{Fe,MEAS}$, $10^{12}$ cm$^{-3}$ | $T$, K | $n_{Fe-FeB}$ | $R_{sh,Fe-FeB}$, Ohm | $n_{Fe}$ | $R_{sh,Fe}$, Ohm | $N_{Fe,PRED}$, $10^{12}$ cm$^{-3}$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | $DNN_{FeFeB}$ | | $DNN_{FeFeB-Fe}$ | |
| | | | | | | | training | full | training | full |
| SC320 | 2.0 ± 0.4 | 300 | 1.214 | $1.6 \cdot 10^6$ | 1.195 | $1.4 \cdot 10^6$ | 3.9 | 2.8 | 3.0 | 2.0 |
| | | 320 | 1.204 | $8.6 \cdot 10^5$ | 1.148 | $8.0 \cdot 10^5$ | 6.6 | 1.9 | 16 | 19 |
| | | 340 | 1.118 | $4.3 \cdot 10^5$ | 1.111 | $4.3 \cdot 10^5$ | 3.8 | 1.2 | 89 | 574 |
| SC349 | 6.7 ± 0.7 | 300 | 1.223 | $2.9 \cdot 10^6$ | 1.222 | $2.6 \cdot 10^6$ | 8.9 | 5.6 | 15 | 11 |
| | | 320 | 1.183 | $1.7 \cdot 10^6$ | 1.182 | $1.7 \cdot 10^6$ | 1.2 | 0.4 | 10 | 32 |
| | | 340 | 1.138 | $1.3 \cdot 10^6$ | 1.173 | $1.3 \cdot 10^6$ | 9.8 | 1.7 | 26 | 411 |