**Extracting the iron concentration in silicon solar cells using photovoltaic parameters and machine learning**

Oleg Olikh, Oleksii Zavhorodnii

*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, Kyiv, 01601, Ukraine*

olegolikh@knu.ua

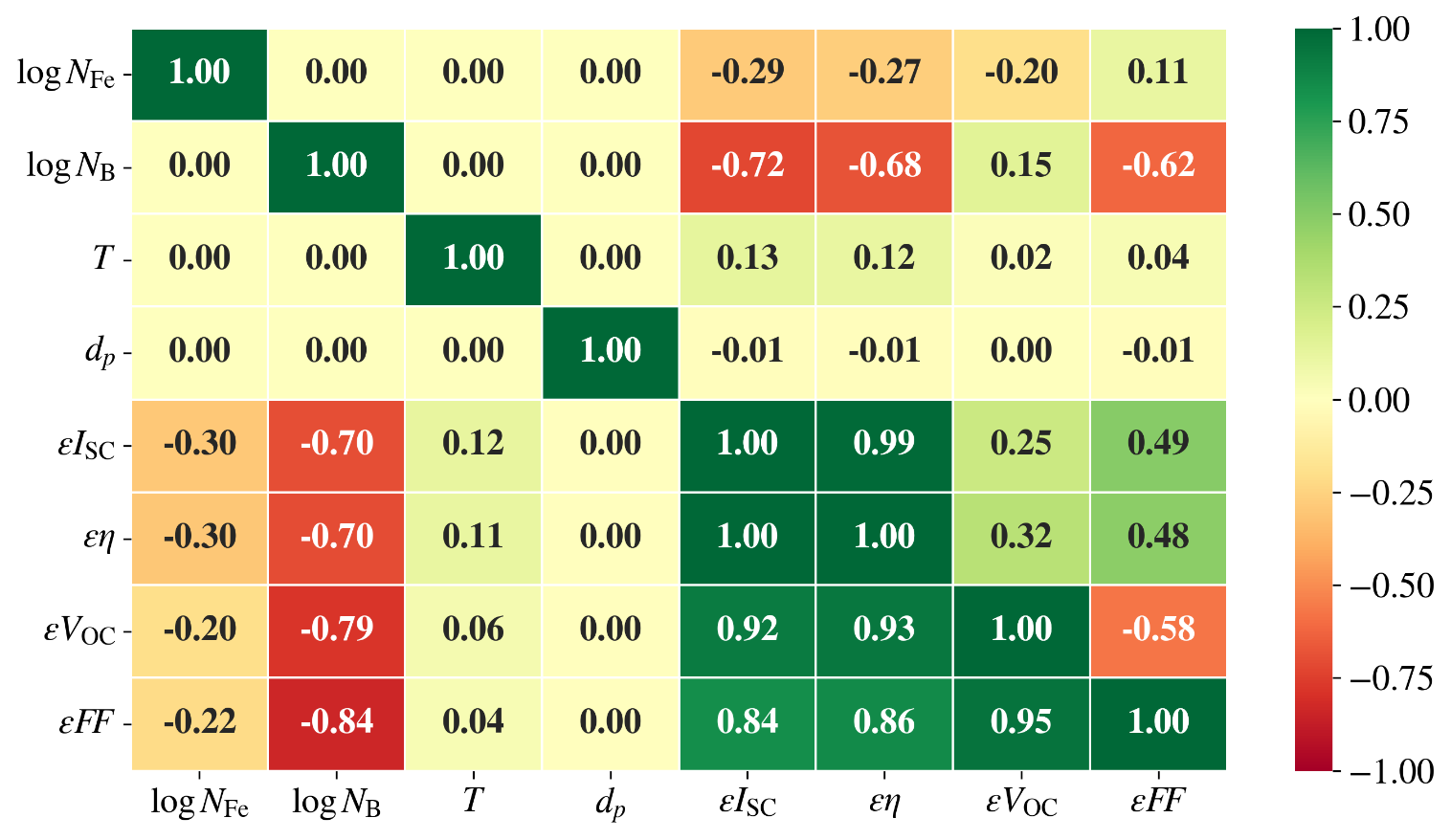


Fig.S1. Correlation plot of features in training set. Data above and below the main diagonal correspond to AM1.5 and 940 nm illumination, respectively.

Table S1. Hyperparameter space for RF

|  |  |
| --- | --- |
| Hyperparameter | Values |
| # estimators | 100, 200, 250, 300, 350, 400, 450,500,550, 600, 650, 700 |
| max depth | 10, 15, 20, 25, 30, 35, 40, 45 |
| min samples leaf | 1, 2, 3, 4, 5, 6, 7 |
| min samples split | 2, 3, 4, 5, 6, 7 |
| bootstrap | True, False |
| max features | 'log2', 'sqrt', 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2 |

Table S2. Hyperparameter space for GB

|  |  |
| --- | --- |
| Hyperparameter | Values |
| # estimators | 100, 200, 250, 300, 350, 400, 450,500,550, 600, 650 |
| max depth | 15, 20, 25, 30, 35, 40, 45 |
| min samples leaf | 1, 2, 3, 4, 5, 6, 7 |
| min samples split | 2, 3, 4, 5, 6, 7 |
| learning rate | [10-3, 10-1] |
| max features | 'log2', 'sqrt', 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2 |

Table S3. Hyperparameter space for XGB

|  |  |
| --- | --- |
| Hyperparameter | Values |
| booster | gbtree, gblinear, dart |
| max depth\* | 3, 4, 5, 6, 7, 10, 15, 20 |
| min split loss\* | [10-6; 5] |
| min child weight\* | [0; 15] |
| subsample\* | 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 |
| сolsample by tree\* | 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 |
| # estimators | 200, 300, 400, 500, 600, 700, 800, 900 |
| learning rate | [10-5; 1] |
| L1 | [10-8; 1] |
| L2 | [10-8; 10] |
| \* for all boosters except gblinear | |

Table S4. Hyperparameter space for SVR

|  |  |
| --- | --- |
| Hyperparameter | Values |
| kernel | linear, poly, rbf, sigmoid |
| degree\* | 2, 3, 4, 5, 6 |
| C0 | [0; 5] |
| Tolerance | [10-5; 10-2] |
| C | [10-2; 15] |
| Epsilon | [10-3; 1] |
| \* for poly kernel only | |

Table S5. Hyperparameter space for DNN

|  |  |
| --- | --- |
| Hyperparameter | Values |
| hidden layers configuration\* | Pipe, Trapezium, Triangle, Butterfly, Fir |
| # nodes for first hidden layer | 5, 10, 20, 30, 50, 75, 100, 120, 150, 200, 250 |
| # hidden layers\*\* | 5, 6, 8, 10, 12, 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; 10-2] |
| # epochs | 100, 300, 400, 500, 600, 700, 1000, 1500 |
| weight initializer | Xavier Normal, Xavier Uniform, He Normal, He Uniform, Random Normal, Random Uniform |
| \* The configurations are shown in Fig.S2. | |
| \*\* For Pipe configuration only | |

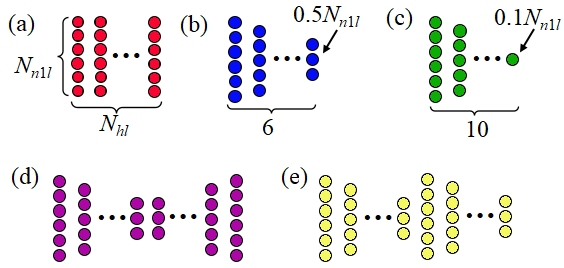
 Fig.S2. The considered configuration of the hidden layers for DNN models: a) pipe; b) trapezium; c) triangle; d) butterfly (two serial reflected trapezium); e) fir (two serial trapezium). *Nn*1*l* is the number nodes for first hidden layer, *Nhl* is the number of hidden layers.

Table S6. Chosen hyperparameter combinations for RF models

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Model | Hyperparameter | | | | | |
| # estimators | max depth | min sample split | min sample leaf | max features | bootstrap |
|  | 200 | 15 | 3 | 1 | 1.0 | True |
|  | 650 | 15 | 2 | 1 | 0.9 | True |
|  | 500 | 30 | 2 | 1 | 0.9 | True |
|  | 200 | 20 | 2 | 1 | 0.9 | True |
|  | 600 | 20 | 2 | 1 | 0.6 | False |
|  | 300 | 15 | 4 | 1 | 0.6 | False |
|  | 500 | 35 | 2 | 1 | 1.0 | True |
|  | 700 | 45 | 2 | 1 | 0.6 | True |
|  | 500 | 30 | 2 | 1 | 0.5 | False |
|  | 600 | 30 | 2 | 1 | 0.6 | False |
|  | 400 | 30 | 2 | 1 | 0.5 | False |
|  | 500 | 25 | 2 | 1 | 0.7 | False |
|  | 600 | 45 | 2 | 1 | 0.7 | False |
|  | 550 | 40 | 2 | 1 | 0.6 | False |
|  | 450 | 40 | 2 | 1 | 0.7 | False |
|  | 450 | 30 | 2 | 1 | 0.6 | False |

Table S7. Chosen hyperparameter combinations for GB models

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Model | Hyperparameter | | | | | |
| # estimators | max depth | min sample split | min sample leaf | max features | learning rate |
|  | 500 | 15 | 4 | 7 | 0.8 | 8.3e-03 |
|  | 550 | 15 | 5 | 7 | 0.8 | 8.1e-03 |
|  | 650 | 30 | 6 | 6 | 0.8 | 1.1e-02 |
|  | 650 | 45 | 4 | 7 | 0.7 | 1.3e-02 |
|  | 650 | 45 | 2 | 4 | 0.8 | 4.3e-02 |
|  | 550 | 15 | 4 | 3 | 0.6 | 7.2e-03 |
|  | 600 | 40 | 4 | 6 | 0.7 | 1.9e-02 |
|  | 600 | 40 | 6 | 6 | 0.5 | 3.8e-02 |
|  | 600 | 45 | 7 | 5 | 0.7 | 3.4e-02 |
|  | 550 | 30 | 7 | 7 | 0.6 | 1.9e-02 |
|  | 650 | 45 | 7 | 7 | 0.7 | 2.7e-02 |
|  | 400 | 35 | 3 | 7 | 0.9 | 3.5e-02 |
|  | 450 | 15 | 4 | 6 | 0.7 | 2.3e-02 |
|  | 550 | 40 | 2 | 6 | 0.6 | 2.1e-02 |
|  | 650 | 15 | 5 | 7 | 0.7 | 2.8e-02 |
|  | 600 | 40 | 3 | 5 | 0.6 | 2.7e-02 |

Table S8. Chosen hyperparameter combinations for XGB models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Model | Hyperparameter | | | | | | | | | |
| booster | max depth | min split loss | min child weight | sub  sample | сolsample bytree | # estimators | learning rate | L1 | L2 |
|  | dart | 10 | 5.3e-4 | 10.8 | 0.6 | 1 | 400 | 1.7e-2 | 2.8e-2 | 3.1e-2 |
|  | gbtree | 15 | 1.9e-3 | 11.1 | 0.7 | 1 | 500 | 9.5e-3 | 1.8e-4 | 2.6e-3 |
|  | dart | 15 | 2.3e-5 | 5.2 | 0.7 | 1 | 700 | 1.1e-2 | 6.6e-3 | 5.3e-2 |
|  | gbtree | 15 | 1.8e-6 | 4 | 0.7 | 1 | 800 | 8.2e-3 | 1.1e-4 | 1 |
|  | gbtree | 15 | 1.1e-5 | 1.9 | 0.7 | 1 | 800 | 7.3e-2 | 9.9e-4 | 9.8 |
|  | dart | 15 | 1.6e-5 | 10.4 | 0.3 | 1 | 800 | 6.7e-3 | 7.0e-3 | 0.5 |
|  | dart | 20 | 1.3e-5 | 1.5 | 0.7 | 1 | 900 | 1.1e-2 | 1.4e-4 | 2.4 |
|  | dart | 20 | 1.3e-4 | 6.9 | 0.6 | 1 | 900 | 1.1e-2 | 2.5e-3 | 1.4e-3 |
|  | dart | 20 | 5.5e-5 | 0.7 | 0.5 | 1 | 500 | 1.7e-2 | 1.7e-3 | 0.3 |
|  | dart | 15 | 6.8e-6 | 5.7 | 0.8 | 1 | 400 | 6.3e-2 | 8.1e-2 | 6.9e-2 |
|  | gbtree | 20 | 1.0e-5 | 3 | 0.5 | 1 | 900 | 1.0e-2 | 7.2e-4 | 1.3e-3 |
|  | dart | 15 | 4.3e-6 | 9.9 | 0.7 | 1 | 500 | 4.7e-2 | 4.9e-4 | 3.3e-2 |
|  | dart | 15 | 1.4e-5 | 3.9 | 0.3 | 1 | 700 | 5.6e-2 | 2.0e-3 | 5.9 |
|  | gbtree | 20 | 4.7e-6 | 12.6 | 0.6 | 0.9 | 900 | 4.4e-2 | 7.9e-2 | 0.3 |
|  | dart | 20 | 2.5e-6 | 8.3 | 0.5 | 1 | 900 | 8.4e-2 | 1.1e-3 | 7.4 |
|  | gbtree | 15 | 1.3e-4 | 1.5 | 0.4 | 1 | 600 | 2.4e-2 | 1.2e-4 | 4.9e-2 |

Table S9. Chosen hyperparameter combinations for SVR models

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | Hyperparameter | | | | |
| kernel | C0 | Tolerance | C | Epsilon |
|  | rbf | 0.78 | 3.3e-05 | 15 | 0.15 |
|  | rbf | 0.81 | 1.1e-03 | 15 | 0.15 |
|  | rbf | 0.31 | 2.3e-03 | 15 | 0.11 |
|  | rbf | 0.81 | 1.4e-03 | 15 | 0.09 |
|  | rbf | 0.56 | 2.7e-04 | 15 | 0.16 |
|  | rbf | 0.88 | 4.5e-03 | 15 | 0.19 |
|  | rbf | 0.67 | 1.8e-04 | 15 | 0.15 |
|  | rbf | 0.69 | 3.8e-04 | 15 | 0.17 |
|  | rbf | 0.35 | 6.3e-03 | 15 | 0.19 |
|  | rbf | 0.11 | 1.9e-04 | 15 | 0.24 |
|  | rbf | 0.94 | 2.9e-04 | 15 | 0.16 |
|  | rbf | 0.42 | 1.7e-04 | 15 | 0.19 |
|  | rbf | 0.42 | 4.8e-04 | 15 | 0.22 |
|  | rbf | 0.02 | 9.5e-04 | 15 | 0.19 |
|  | rbf | 0.82 | 7.2e-04 | 15 | 0.19 |
|  | rbf | 0.95 | 1.2e-04 | 15 | 0.17 |

Table S10. Chosen hyperparameter combinations for DNN models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Мережа | Параметр | | | | | | | | | |
| config | *Nhl* | *Nn*1*l* | BS | Epochs | LR, 10-4 | Optim | Activ | Init |
|  | Pipe | 8 | 50 | 64 | 500 | 12.0 | Adamax | tanh | XN |
|  | Pipe | 8 | 120 | 16 | 500 | 5.4 | Nadam | tanh | XU |
|  | Pipe | 5 | 200 | 128 | 500 | 3.4 | Nadam | tanh | XU |
|  | Trapezium | - | 250 | 16 | 500 | 3.7 | Adamax | tanh | XN |
|  | Trapezium | - | 50 | 16 | 500 | 2.7 | Adam | tanh | XN |
|  | Pipe | 10 | 50 | 16 | 500 | 6.3 | Adamax | relu | XN |
|  | Trapezium | - | 200 | 64 | 500 | 7.8 | Adamax | tanh | XU |
|  | Pipe | 5 | 100 | 16 | 500 | 1.9 | Adamax | relu | XN |
|  | Trapezium | - | 150 | 8 | 500 | 3.5 | Nadam | tanh | XN |
|  | Trapezium | - | 150 | 128 | 500 | 1.5 | Nadam | tanh | XU |
|  | Pipe | 5 | 50 | 128 | 500 | 3.9 | Nadam | elu | XU |
|  | Trapezium | - | 150 | 64 | 500 | 1.0 | Nadam | tanh | XU |
|  | Pipe | 5 | 120 | 16 | 500 | 10.3 | Adamax | elu | XN |
|  | Trapezium | - | 100 | 32 | 500 | 18.3 | Adamax | relu | XN |
|  | Pipe | 6 | 50 | 16 | 500 | 16.4 | Nadam | tanh | XN |
|  | Pipe | 6 | 100 | 8 | 500 | 60.5 | Adamax | elu | XU |

Table S11. Performance metrics of the models using fivefold cross-validation of train dataset

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | MAPE, % | R2, 10-3 | Model | MSE, 10-3 | MAPE, % | R2, 10-3 |
|  | 5.2 ± 0.1 | 11 ± 2 | 980 ± 5 |  | 32 ± 3 | 41 ± 7 | 970 ± 10 |
|  | 7.0 ± 1.0 | 12 ± 1 | 976 ± 4 |  | 52 ± 5 | 90 ± 30 | 910 ± 10 |
|  | 4.1 ± 0.5 | 9.6 ± 0.5 | 994 ± 1 |  | 12 ± 2 | 17 ± 3 | 993 ± 3 |
|  | 6 ± 1 | 13 ± 1 | 970 ± 10 |  | 76 ± 6 | 100 ± 20 | 895 ± 15 |
|  | 3.0 ± 0.8 | 7.1 ± 0.5 | 997 ± 2 |  | 4.3 ± 0.4 | 7.9 ± 0.5 | 994 ± 4 |
|  | 6 ± 1 | 14 ± 4 | 971 ± 8 |  | 25 ± 5 | 34 ± 10 | 940 ± 15 |
|  | 3.0 ± 0.8 | 6.6 ± 0.3 | **998 ± 1** |  | 3.9 ± 0.4 | 7.0 ± 0.7 | 994 ± 6 |
|  | 3.6 ± 0.9 | 9.0 ± 0.5 | 993 ± 2 |  | 7 ± 1 | 12 ± 1 | 966 ± 5 |
|  | 3.7 ± 0.9 | 7.4 ± 0.7 | 986 ± 3 |  | 34 ± 6 | 60 ± 20 | 940 ± 7 |
|  | 5.0 ± 0.9 | 10 ± 1 | 975 ± 8 |  | 55 ± 8 | 100 ± 30 | 910 ± 10 |
|  | 2.5 ± 0.5 | 6.5 ± 0.2 | 995 ± 1 |  | 10 ± 2 | 14 ± 4 | 993 ± 3 |
|  | 4 ± 1 | 9.4 ± 0.7 | 983 ± 4 |  | 77 ± 7 | 130 ± 10 | 900 ± 15 |
|  | 1.9 ± 0.3 | 5.2 ± 0.3 | 997 ± 1 |  | 4.1 ± 0.6 | 7.7 ± 0.9 | **997 ± 2** |
|  | 5 ± 1 | 11 ± 4 | 976 ± 7 |  | 23 ± 4 | 30 ± 10 | 937 ± 7 |
|  | 1.9 ± 0.2 | 5.3 ± 0.3 | **998 ± 1** |  | 3.3 ± 0.6 | 6.5 ± 0.4 | 992 ± 4 |
|  | 3.2 ± 0.6 | 8.0 ± 0.6 | 992 ± 3 |  | 5.4 ± 0.9 | 9.6 ± 0.5 | 970 ± 10 |
|  | 4.8 ± 0.5 | 9.2 ± 0.8 | 964 ± 4 |  | 36 ± 4 | 50 ± 10 | 925 ± 15 |
|  | 8.7 ± 0.5 | 15 ± 1 | 960 ± 6 |  | 52 ± 5 | 110 ± 50 | 900 ± 10 |
|  | 2.8 ± 0.4 | 6.4 ± 0.4 | 982 ± 4 |  | 10 ± 2 | 19 ± 7 | 985 ± 2 |
|  | 6.5 ± 0.4 | 11.2 ± 0.3 | 966 ± 6 |  | 80 ± 4 | 130 ± 30 | 870 ± 10 |
|  | **1.4 ± 0.3** | **4.3 ± 0.3** | 996 ± 1 |  | 3.3 ± 0.5 | 6.8 ± 0.7 | **997 ± 3** |
|  | 5.8 ± 0.9 | 11 ± 1 | 968 ± 6 |  | 22 ± 2 | 35 ± 10 | 950 ± 10 |
|  | 1.5 ± 0.2 | 5.4 ± 0.1 | 996 ± 1 |  | 2.7 ± 0.3 | 6.5 ± 0.6 | 992 ± 4 |
|  | 4 ± 1 | 8.1 ± 0.5 | 970 ± 20 |  | 5 ± 1 | 10 ± 1 | 961 ± 7 |
|  | 220 ± 20 | 200 ± 20 | 540 ± 30 |  | 230 ± 5 | 220 ± 20 | 500 ± 20 |
|  | 221 ± 7 | 205 ± 15 | 530 ± 40 |  | 230 ± 10 | 215 ± 10 | 510 ± 20 |
|  | 210 ± 10 | 180 ± 15 | 480 ± 40 |  | 200 ± 10 | 180 ± 30 | 520 ± 20 |
|  | 215 ± 9 | 180 ± 15 | 520 ± 20 |  | 243 ± 8 | 220 ± 8 | 500 ± 20 |
|  | 180 ± 7 | 127 ± 7 | 600 ± 10 |  | 180 ± 15 | 59 ± 2 | 420 ± 30 |
|  | 204 ± 8 | 150 ± 10 | 515 ± 20 |  | 210 ± 15 | 76 ± 4 | 300 ± 60 |
|  | 161 ± 9 | 115 ± 10 | 610 ± 30 |  | 140 ± 8 | 55 ± 1 | 390 ± 60 |
|  | 188 ± 9 | 124 ± 8 | 600 ± 20 |  | 140 ± 9 | 50 ± 1 | 450 ± 10 |
|  | 6 ± 1 | 10 ± 2 | 971 ± 3 |  | 38 ± 4 | 57 ± 3 | 940 ± 10 |
|  | 6 ± 2 | 9 ± 2 | 980 ± 10 |  | 80 ± 20 | 125 ± 40 | 860 ± 30 |
|  | 6 ± 1 | 11 ± 2 | 970 ± 7 |  | 9 ± 6 | 25 ± 15 | 985 ± 5 |
|  | 7 ± 2 | 12 ± 3 | 973 ± 6 |  | 80 ± 8 | 230 ± 110 | 930 ± 15 |
|  | 4 ± 1 | 11 ± 3 | 970 ± 9 |  | 10 ± 6 | 14 ± 5 | 980 ± 15 |
|  | 5 ± 2 | 12 ± 7 | 967 ± 6 |  | 2.2 ± 0.7 | 7 ± 2 | 994 ± 4 |
|  | 20 ± 10 | 45 ± 25 | 880 ± 100 |  | **0.8 ± 0.4** | 3.2 ± 0.7 | 997 ± 2 |
|  | 15 ± 10 | 14 ± 2 | 975 ± 7 |  | 0.9 ± 0.5 | **3 ± 1** | 997 ± 2 |

Table S12. Performance metrics of the models for train dataset. Illumination 940 nm.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | R2 | MAPE, % | MedAPE, % | *p*01, % | *p*10, % |
|  | 0.60 | 0.9979 | 3.11 | 1.468 | 39.85 | 95.37 |
|  | 1.05 | 0.99639 | 4.20 | 2.134 | 32.19 | 91.22 |
|  | 0.444 | 0.99976 | 2.91 | 1.077 | 48.39 | 94.63 |
|  | 0.662 | 0.9967 | 3.89 | 2.174 | 29.56 | 92.1 |
|  | 0 | 1.000 | 0.002 | 8.17E-13 | 100 | 100 |
|  | 0.0036 | 0.999 | 0.045 | 8.203E-13 | 99.47 | 99.91 |
|  | 0 | 1.000 | 0 | 8.184E-13 | 100 | 100 |
|  | 0 | 1.000 | 0.0026 | 8.184E-13 | 99.96 | 100 |
|  | 0.499 | 0.99725 | 0.160 | 0.5048 | 71.02 | 97.87 |
|  | 0.47 | 0. 9977 | 1.52 | 0.4638 | 72.64 | 97.98 |
|  | 0.0402 | 0.99970 | 0.604 | 0.2315 | 87.26 | 99.47 |
|  | 0.0087 | 0.99993 | 0.36 | 0.1678 | 93.65 | 99.93 |
|  | 0.0058 | 0.999 | 0.26 | 0.1112 | 95.68 | 99.98 |
|  | 0.0370 | 0. 99970 | 0.599 | 0.2469 | 86.68 | 99.56 |
|  | 0.0119 | 0.99992 | 0.50 | 0.2419 | 87.62 | 99.9 |
|  | 0.0007 | 1.000 | 0.107 | 0.05002 | 99.14 | 100 |
|  | 2.282 | 0.98091 | 4.64 | 1.559 | 36 | 92.15 |
|  | 3.929 | 0.9846 | 7.41 | 2.17 | 30.5 | 82.72 |
|  | 0.788 | 0.99490 | 1.94 | 0.617 | 66.3 | 97.31 |
|  | 3.729 | 0.9857 | 6.56 | 1.85 | 32.43 | 88.35 |
|  | 0.174 | 0.99954 | 1.060 | 0.4432 | 76.06 | 98.93 |
|  | 1.97 | 0.9924 | 4.63 | 1.645 | 34.76 | 91.14 |
|  | 0.052 | 0.99983 | 0.84 | 0.4336 | 77.72 | 99.52 |
|  | 0.35 | 0.9992 | 2.01 | 1.156 | 44.52 | 98.1 |
|  | 215 | 0.549 | 201 | 33.24 | 1.358 | 15.48 |
|  | 215 | 0.537 | 200 | 29.55 | 1.673 | 17.46 |
|  | 204 | 0.492 | 171 | 34.94 | 1.552 | 15.05 |
|  | 210 | 0.535 | 177 | 40.48 | 1.139 | 12.77 |
|  | 174 | 0.609 | 124 | 35.86 | 1.608 | 13.71 |
|  | 199 | 0.548 | 142 | 41.63 | 1.277 | 11.81 |
|  | 155 | 0.626 | 112 | 37.34 | 1.188 | 12.42 |
|  | 182 | 0.628 | 122 | 36.34 | 1.349 | 14.22 |
|  | 5 | 0.962 | 12 | 6.787 | 7.717 | 67.28 |
|  | 11 | 0.952 | 17 | 7.833 | 6.804 | 60.34 |
|  | 8 | 0.963 | 12 | 5.977 | 8.727 | 72.91 |
|  | 8 | 0.940 | 17 | 6.983 | 7.572 | 65.73 |
|  | 4 | 0.966 | 9 | 5.205 | 10.26 | 75.68 |
|  | 4 | 0.958 | 9 | 4.611 | 12.86 | 77.29 |
|  | 12 | 0.931 | 24 | 14.4 | 4.186 | 38.54 |
|  | 4 | 0.983 | 8 | 5.109 | 10.03 | 77.92 |

Table S13. Performance metrics of the models for train dataset. Illumination AM1.5.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | R2 | MAPE, % | MedAPE, % | *p*01, % | *p*10, % |
|  | 15.7 | 0.986 | 16.3 | 2.264 | 37.96 | 78.81 |
|  | 27.6 | 0.9407 | 30.9 | 3.939 | 18.95 | 73.54 |
|  | 0.25 | 0.99993 | 1.0 | 0.1921 | 90.97 | 98.26 |
|  | 43.1 | 0.929 | 44.1 | 3.89 | 24.28 | 68.2 |
|  | 0.0009 | 0.99999 | 0.1 | 8.107E-13 | 100 | 100 |
|  | 0.0008 | 1.000 | 0.0032 | 1.635E-12 | 98.95 | 100 |
|  | 0 | 1.000 | 0 | 1.234E-12 | 100 | 100 |
|  | 0 | 1.000 | 0 | 8.184E-13 | 100 | 100 |
|  | 12.9 | 0.9693 | 16.3 | 4.521 | 10.55 | 81.41 |
|  | 19.4 | 0.9559 | 21.9 | 3.506 | 14.34 | 82.42 |
|  | 0 | 1.000 | 0.008 | 0.002666 | 100 | 100 |
|  | 20.3 | 0.9586 | 23.4 | 6.337 | 7.232 | 70.86 |
|  | 0.0002 | 1.000 | 0.0027 | 0.007811 | 99.77 | 100 |
|  | 0.00142 | 0.99858 | 1.01 | 0.3292 | 80.75 | 98.55 |
|  | 0.026 | 0.99984 | 0.48 | 0.1894 | 89.64 | 99.77 |
|  | 0.0078 | 0. 99971 | 0.197 | 0.08304 | 97.52 | 99.88 |
|  | 24.2 | 0.9465 | 26.9 | 4.362 | 14.63 | 73.26 |
|  | 32.3 | 0.933 | 43.9 | 4.954 | 12.61 | 69.65 |
|  | 1.820 | 0.99777 | 1.158 | 0.541 | 73.43 | 98.59 |
|  | 55.0 | 0.906 | 66.4 | 7.317 | 9.891 | 57.49 |
|  | 0.025 | 0.999 | 0.897 | 0.6342 | 68.15 | 99.85 |
|  | 0.161 | 0.9983 | 2.27 | 1.592 | 33.94 | 98.52 |
|  | 0.17 | 0.9991 | 1.38 | 0.731 | 61.61 | 98.93 |
|  | 0.154 | 0.9979 | 2.04 | 1.389 | 38.34 | 98.63 |
|  | 225 | 0.520 | 209 | 42.62 | 1.131 | 11.71 |
|  | 224 | 0.521 | 209 | 41.86 | 1.366 | 12.08 |
|  | 197 | 0.551 | 181 | 38.96 | 1.244 | 11.14 |
|  | 238 | 0.525 | 213 | 50.62 | 0.897 | 9.939 |
|  | 170 | 0.465 | 56 | 38.36 | 1.261 | 11.85 |
|  | 202 | 0.336 | 74 | 46.59 | 0.9212 | 9.228 |
|  | 133 | 0.444 | 53 | 38.09 | 1.172 | 12.66 |
|  | 133 | 0.504 | 49 | 34.6 | 1.584 | 14.17 |
|  | 31 | 0.936 | 37 | 10.17 | 5.067 | 49.32 |
|  | 47 | 0.870 | 61 | 14.32 | 3.79 | 36.55 |
|  | 8 | 0.987 | 61 | 5.279 | 10.41 | 75.47 |
|  | 48 | 0.941 | 57 | 6.544 | 9.156 | 63.31 |
|  | 6 | 0.979 | 11 | 5.287 | 10.69 | 75.45 |
|  | 2 | 0.995 | 5 | 3.01 | 19.61 | 92.74 |
|  | 0.3 | 0.998 | 3 | 1.747 | 29.81 | 98 |
|  | 0.4 | 0.998 | 3 | 2.146 | 24.64 | 97.9 |

Table S11. Performance metrics of the models for train dataset

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | MAPE, % | R2 | Model | MSE, 10-3 | MAPE, % | R2 |
|  | 0.60 ± 0.01 | 3.11 ± 0.01 | 0.9979 ± 0.0001 |  | 15.7 ± 0.2 | 16.3 ± 0.2 | 0.986 ± 0.001 |
|  | 1.05 ± 0.02 | 4.20 ± 0.02 | 0.99639 ± 0.00004 |  | 27.6 ± 0.1 | 30.9 ± 0.1 | 0.9407 ± 0.0004 |
|  | 0.444 ± 0.003 | 2.91 ± 0.01 | 0.99976 ± 0.00001 |  | 0.25 ± 0.01 | 1.0 ± 0.1 | 0.99993 ± 0.00004 |
|  | 0.662 ± 0.004 | 3.89 ± 0.01 | 0.9967 ± 0.0001 |  | 43.1 ± 0.2 | 44.1 ± 0.4 | 0.929 ± 0.001 |
|  | 0 | 0.002 ± 0.002 | 1.000 |  | 0.0009 ± 0.0004 | 0.1 ± 0.1 | 0.99999 ± 0.00002 |
|  | 0.0036 ± 0.0005 | 0.045 ± 0.003 | 0.999 |  | 0.0008 ± 0.0002 | 0.0032 ± 0.0004 | 1.000 |
|  | 0 | 0 | 1.000 |  | 0 | 0 | 1.000 |
|  | 0 | 0.0026 ± 0.0004 | 1.000 |  | 0 | 0 | 1.000 |
|  | 0.499 ± 0.003 | 0.160 ± 0.003 | 0.99725 ± 0.00002 |  | 12.9 ± 0.1 | 16.3 ± 0.1 | 0.9693 ± 0.0002 |
|  | 0.47 ± 0.01 | 1.52 ± 0.01 | 0. 9977 ± 0.0001 |  | 19.4 ± 0.1 | 21.9 ± 0.2 | 0.9559 ± 0.0004 |
|  | 0.0402 ± 0.0007 | 0.604 ± 0.004 | 0.99970 ± 0.00001 |  | 0 | 0.008 ± 0.001 | 1.000 |
|  | 0.0087 ± 0.0004 | 0.36 ± 0.01 | 0.99993 ± 0.00001 |  | 20.3 ± 0.1 | 23.4 ± 0.1 | 0.9586 ± 0.0004 |
|  | 0.0058 ± 0.0002 | 0.26 ± 0.01 | 0.999 |  | 0.0002 | 0.0027 ± 0.0001 | 1.000 |
|  | 0.0370 ± 0.0005 | 0.599 ± 0.002 | 0. 99970 ± 0.00002 |  | 0.00142 ± 0.00003 | 1.01 ± 0.01 | 0.99858 ± 0.00004 |
|  | 0.0119 ± 0.0004 | 0.50 ± 0.01 | 0.99992 ± 0.00001 |  | 0.026 ± 0.001 | 0.48 ± 0.01 | 0.99984 ± 0.00003 |
|  | 0.0007 | 0.107 ± 0.002 | 1.000 |  | 0.0078 ± 0.0004 | 0.197 ± 0.004 | 0. 99971 ± 0.00003 |
|  | 2.282 ± 0.0004 | 4.64 ± 0.01 | 0.98091 ± 0.00004 |  | 24.2 ± 0.08 | 26.9 ± 0.2 | 0.9465 ± 0.0002 |
|  | 3.929 ± 0.0003 | 7.41 ± 0.01 | 0.9846 ± 0.0001 |  | 32.3 ± 0.03 | 43.9 ± 0.5 | 0.933 ± 0.001 |
|  | 0.788 ± 0.004 | 1.94 ± 0.01 | 0.99490 ± 0.00002 |  | 1.820 ± 0.004 | 1.158 ± 0.0002 | 0.99777 ± 0.00001 |
|  | 3.729 ± 0.006 | 6.56 ± 0.02 | 0.9857 ± 0.0001 |  | 55.0 ± 0.1 | 66.4 ± 0.7 | 0.906 ± 0.001 |
|  | 0.174 ± 0.004 | 1.060 ± 0.003 | 0.99954 ± 0.00004 |  | 0.025 ± 0.001 | 0.897 ± 0.004 | 0.999 |
|  | 1.97 ± 0.01 | 4.63 ± 0.03 | 0.9924 ± 0.0001 |  | 0.161 ± 0.003 | 2.27 ± 0.02 | 0.9983 ± 0.0001 |
|  | 0.052 ± 0.001 | 0.84 ± 0.01 | 0.99983 ± 0.00001 |  | 0.17 ± 0.01 | 1.38 ± 0.02 | 0.9991 ± 0.0002 |
|  | 0.35 ± 0.01 | 2.01 ± 0.02 | 0.9992 ± 0.0001 |  | 0.154 ± 0.004 | 2.04 ± 0.01 | 0.9979 ± 0.0001 |
|  | 215 | 201 | 0.549 |  | 225 | 209 | 0.520 |
|  | 215 | 200 | 0.537 |  | 224 | 209 | 0.521 |
|  | 204 | 171 | 0.492 |  | 197 | 181 | 0.551 |
|  | 210 | 177 | 0.535 |  | 238 | 213 | 0.525 |
|  | 174 | 124 | 0.609 |  | 170 | 56 | 0.465 |
|  | 199 | 142 | 0.548 |  | 202 | 74 | 0.336 |
|  | 155 | 112 | 0.626 |  | 133 | 53 | 0.444 |
|  | 182 | 122 | 0.628 |  | 133 | 49 | 0.504 |
|  | 5 | 12 | 0.962 |  | 31 | 37 | 0.936 |
|  | 11 | 17 | 0.952 |  | 47 | 61 | 0.870 |
|  | 8 | 12 | 0.963 |  | 8 | 61 | 0.987 |
|  | 8 | 17 | 0.940 |  | 48 | 57 | 0.941 |
|  | 4 | 9 | 0.966 |  | 6 | 11 | 0.979 |
|  | 4 | 9 | 0.958 |  | 2 | 5 | 0.995 |
|  | 12 | 24 | 0.931 |  | 0.3 | 3 | 0.998 |
|  | 4 | 8 | 0.983 |  | 0.4 | 3 | 0.998 |

Table S12. Performance metrics of the models for train dataset

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | MAPE, % | R2 | Model | MSE, 10-3 | MAPE, % | R2 |
|  | 0.60 | 3.11 | 0.9979 |  | 15.7 | 16.3 | 0.986 |
|  | 1.05 | 4.20 | 0.99639 |  | 27.6 | 30.9 | 0.9407 |
|  | 0.444 | 2.91 | 0.99976 |  | 0.25 | 1.0 | 0.99993 |
|  | 0.662 | 3.89 | 0.9967 |  | 43.1 | 44.1 | 0.929 |
|  | 0 | 0.002 | 1.000 |  | 0.0009 | 0.1 | 0.99999 |
|  | 0.0036 | 0.045 | 0.999 |  | 0.0008 | 0.0032 | 1.000 |
|  | 0 | 0 | 1.000 |  | 0 | 0 | 1.000 |
|  | 0 | 0.0026 | 1.000 |  | 0 | 0 | 1.000 |
|  | 0.499 | 0.160 | 0.99725 |  | 12.9 | 16.3 | 0.9693 |
|  | 0.47 | 1.52 | 0. 9977 |  | 19.4 | 21.9 | 0.9559 |
|  | 0.0402 | 0.604 | 0.99970 |  | 0 | 0.008 | 1.000 |
|  | 0.0087 | 0.36 | 0.99993 |  | 20.3 | 23.4 | 0.9586 |
|  | 0.0058 | 0.26 | 0.999 |  | 0.0002 | 0.0027 | 1.000 |
|  | 0.0370 | 0.599 | 0. 99970 |  | 0.00142 | 1.01 | 0.99858 |
|  | 0.0119 | 0.50 | 0.99992 |  | 0.026 | 0.48 | 0.99984 |
|  | 0.0007 | 0.107 | 1.000 |  | 0.0078 | 0.197 | 0. 99971 |
|  | 2.282 | 4.64 | 0.98091 |  | 24.2 | 26.9 | 0.9465 |
|  | 3.929 | 7.41 | 0.9846 |  | 32.3 | 43.9 | 0.933 |
|  | 0.788 | 1.94 | 0.99490 |  | 1.820 | 1.158 | 0.99777 |
|  | 3.729 | 6.56 | 0.9857 |  | 55.0 | 66.4 | 0.906 |
|  | 0.174 | 1.060 | 0.99954 |  | 0.025 | 0.897 | 0.999 |
|  | 1.97 | 4.63 | 0.9924 |  | 0.161 | 2.27 | 0.9983 |
|  | 0.052 | 0.84 | 0.99983 |  | 0.17 | 1.38 | 0.9991 |
|  | 0.35 | 2.01 | 0.9992 |  | 0.154 | 2.04 | 0.9979 |
|  | 215 | 201 | 0.549 |  | 225 | 209 | 0.520 |
|  | 215 | 200 | 0.537 |  | 224 | 209 | 0.521 |
|  | 204 | 171 | 0.492 |  | 197 | 181 | 0.551 |
|  | 210 | 177 | 0.535 |  | 238 | 213 | 0.525 |
|  | 174 | 124 | 0.609 |  | 170 | 56 | 0.465 |
|  | 199 | 142 | 0.548 |  | 202 | 74 | 0.336 |
|  | 155 | 112 | 0.626 |  | 133 | 53 | 0.444 |
|  | 182 | 122 | 0.628 |  | 133 | 49 | 0.504 |
|  | 5 | 12 | 0.962 |  | 31 | 37 | 0.936 |
|  | 11 | 17 | 0.952 |  | 47 | 61 | 0.870 |
|  | 8 | 12 | 0.963 |  | 8 | 61 | 0.987 |
|  | 8 | 17 | 0.940 |  | 48 | 57 | 0.941 |
|  | 4 | 9 | 0.966 |  | 6 | 11 | 0.979 |
|  | 4 | 9 | 0.958 |  | 2 | 5 | 0.995 |
|  | 12 | 24 | 0.931 |  | 0.3 | 3 | 0.998 |
|  | 4 | 8 | 0.983 |  | 0.4 | 3 | 0.998 |

Table S11. Performance metrics of the models using fivefold cross-validation of train dataset

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Model | MSE, 10-3 | MAPE, % | R2 | Model | MSE, 10-3 | MAPE, % | R2 |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |