**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

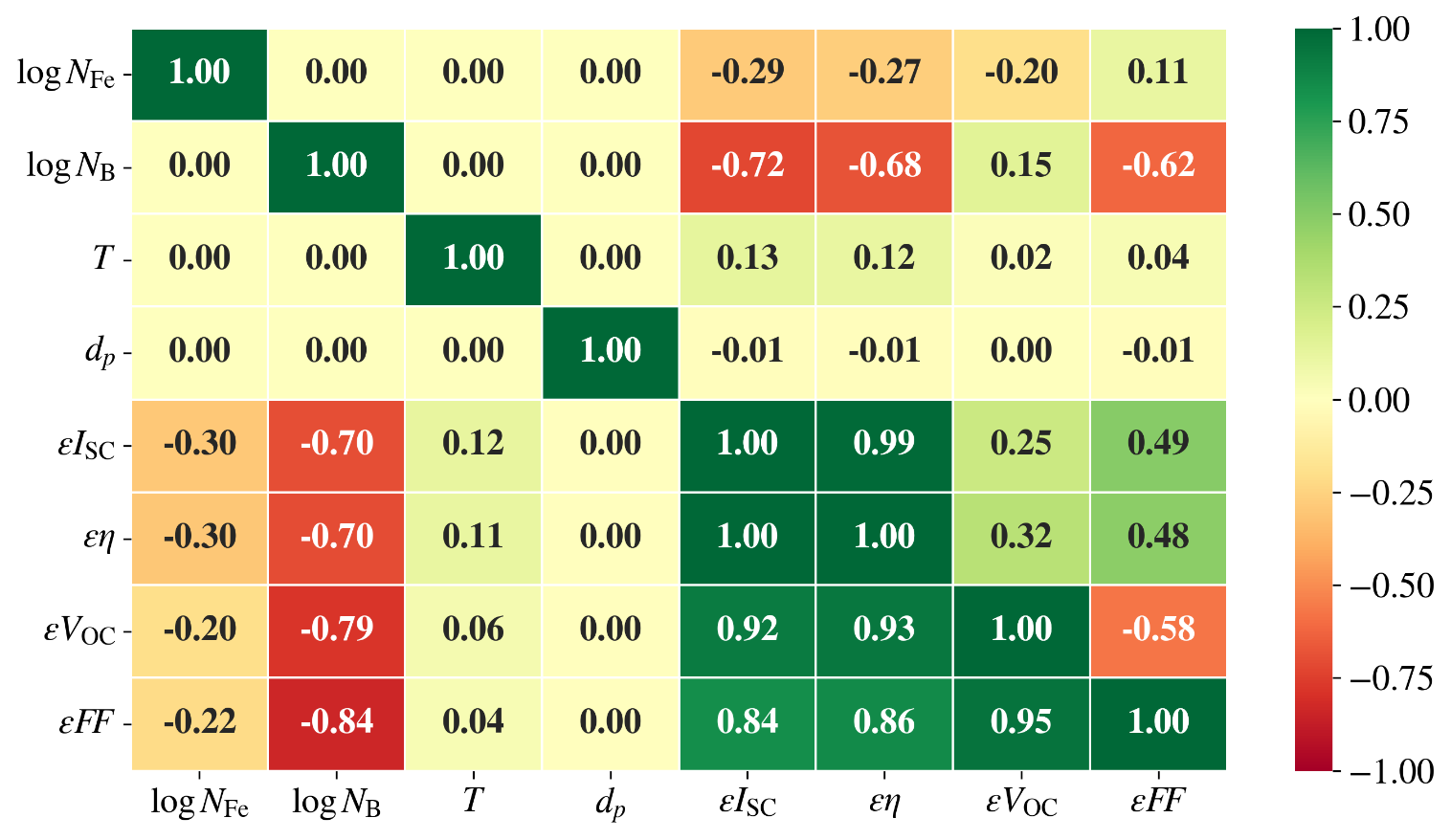


Fig.S1. Correlation plot of features in training set. Data above and below the main diagonal correspond to AM1.5 and 940 nm illumination, respectively.

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 | |

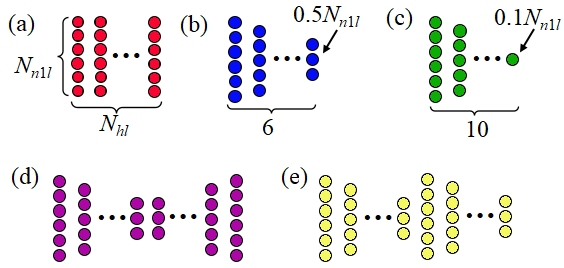
 Fig.S2. The considered configuration of the hidden layers for DNN models: a) pipe; b) trapezium; c) triangle; d) butterfly (two serial reflected trapezium); e) fir (two serial trapezium). *Nn*1*l* is the number nodes for first hidden layer, *Nhl* is the number of hidden layers.

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 |
|  | ± | ± | ± |  | 230 ± 5 | 220 ± 20 | 500 ± 20 |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | 200 ± 10 | 180 ± 30 | 520 ± 20 |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | 180 ± 15 | 59 ± 2 | 420 ± 30 |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | 140 ± 8 | 55 ± 1 | 390 ± 60 |
|  | ± | ± | ± |  | ± | ± | ± |
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|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |

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 |
|  | 52 ± 1 | ± | ± |  | ± | ± | ± |
|  | ± | ± | ± |  | ± | ± | ± |
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