

**Supplementary Table S3.**

Optimization results for GSE154762 dataset of the baseline methods with the different combination of the parameters.

Grid search was adopted for the model tuning, and the hyperparameters showing the best accuracy were selected.

Row with the bolded font are the hyperparameters selected.

| <b>Support vector machine (SVM)</b> |                       |                             |          |
|-------------------------------------|-----------------------|-----------------------------|----------|
| Kernel                              | Penalty parameter (C) | RBF kernel coeff<br>(Gamma) | Accruacy |
| RBF                                 | $2^{-5}$              | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^{-5}$              | $2^{-13}$                   | 0.3000   |
| RBF                                 | $2^{-5}$              | $2^{-11}$                   | 0.3000   |
| RBF                                 | $2^{-5}$              | $2^{-9}$                    | 0.3000   |
| RBF                                 | $2^{-5}$              | $2^{-7}$                    | 0.2963   |
| RBF                                 | $2^{-5}$              | $2^{-5}$                    | 0.4667   |
| RBF                                 | $2^{-5}$              | $2^{-3}$                    | 0.4593   |
| RBF                                 | $2^{-5}$              | $2^{-1}$                    | 0.2148   |
| RBF                                 | $2^{-5}$              | $2^1$                       | 0.1889   |
| RBF                                 | $2^{-5}$              | $2^3$                       | 0.2630   |
| RBF                                 | $2^{-3}$              | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^{-3}$              | $2^{-13}$                   | 0.3000   |
| RBF                                 | $2^{-3}$              | $2^{-11}$                   | 0.3000   |
| RBF                                 | $2^{-3}$              | $2^{-9}$                    | 0.3000   |
| RBF                                 | $2^{-3}$              | $2^{-7}$                    | 0.5111   |
| RBF                                 | $2^{-3}$              | $2^{-5}$                    | 0.6000   |
| RBF                                 | $2^{-3}$              | $2^{-3}$                    | 0.5333   |
| RBF                                 | $2^{-3}$              | $2^{-1}$                    | 0.2556   |
| RBF                                 | $2^{-3}$              | $2^1$                       | 0.1889   |
| RBF                                 | $2^{-3}$              | $2^3$                       | 0.2630   |
| RBF                                 | $2^{-1}$              | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^{-1}$              | $2^{-13}$                   | 0.3000   |
| RBF                                 | $2^{-1}$              | $2^{-11}$                   | 0.3000   |
| RBF                                 | $2^{-1}$              | $2^{-9}$                    | 0.5074   |
| RBF                                 | $2^{-1}$              | $2^{-7}$                    | 0.6667   |
| RBF                                 | $2^{-1}$              | $2^{-5}$                    | 0.7148   |
| RBF                                 | $2^{-1}$              | $2^{-3}$                    | 0.7148   |
| RBF                                 | $2^{-1}$              | $2^{-1}$                    | 0.3778   |
| RBF                                 | $2^{-1}$              | $2^1$                       | 0.1889   |
| RBF                                 | $2^{-1}$              | $2^3$                       | 0.2630   |
| RBF                                 | $2^0$                 | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^0$                 | $2^{-13}$                   | 0.3000   |
| RBF                                 | $2^0$                 | $2^{-11}$                   | 0.4333   |
| RBF                                 | $2^0$                 | $2^{-9}$                    | 0.5778   |
| RBF                                 | $2^0$                 | $2^{-7}$                    | 0.7000   |
| RBF                                 | $2^0$                 | $2^{-5}$                    | 0.7407   |
| RBF                                 | $2^0$                 | $2^{-3}$                    | 0.8333   |
| RBF                                 | $2^0$                 | $2^{-1}$                    | 0.4667   |
| RBF                                 | $2^0$                 | $2^1$                       | 0.2111   |
| RBF                                 | $2^0$                 | $2^3$                       | 0.1963   |
| RBF                                 | $2^1$                 | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^1$                 | $2^{-13}$                   | 0.3000   |
| RBF                                 | $2^1$                 | $2^{-11}$                   | 0.5074   |
| RBF                                 | $2^1$                 | $2^{-9}$                    | 0.6778   |
| RBF                                 | $2^1$                 | $2^{-7}$                    | 0.7148   |
| RBF                                 | $2^1$                 | $2^{-5}$                    | 0.8185   |
| RBF                                 | $2^1$                 | $2^{-3}$                    | 0.8407   |
| RBF                                 | $2^1$                 | $2^{-1}$                    | 0.5037   |
| RBF                                 | $2^1$                 | $2^1$                       | 0.2074   |
| RBF                                 | $2^1$                 | $2^3$                       | 0.1815   |
| RBF                                 | $2^3$                 | $2^{-15}$                   | 0.3000   |
| RBF                                 | $2^3$                 | $2^{-13}$                   | 0.5111   |
| RBF                                 | $2^3$                 | $2^{-11}$                   | 0.6815   |
| RBF                                 | $2^3$                 | $2^{-9}$                    | 0.7148   |

|            |                      |                       |               |
|------------|----------------------|-----------------------|---------------|
| RBF        | 2 <sup>3</sup>       | 2 <sup>-7</sup>       | 0.8185        |
| RBF        | 2 <sup>3</sup>       | 2 <sup>-5</sup>       | 0.8481        |
| RBF        | 2 <sup>3</sup>       | 2 <sup>-3</sup>       | 0.8407        |
| RBF        | 2 <sup>3</sup>       | 2 <sup>-1</sup>       | 0.5037        |
| RBF        | 2 <sup>3</sup>       | 2 <sup>1</sup>        | 0.2074        |
| RBF        | 2 <sup>3</sup>       | 2 <sup>3</sup>        | 0.1815        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-15</sup>      | 0.5111        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-13</sup>      | 0.6815        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-11</sup>      | 0.7185        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-9</sup>       | 0.8074        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-7</sup>       | 0.8481        |
| <b>RBF</b> | <b>2<sup>5</sup></b> | <b>2<sup>-5</sup></b> | <b>0.8593</b> |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-3</sup>       | 0.8407        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>-1</sup>       | 0.5037        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>1</sup>        | 0.2074        |
| RBF        | 2 <sup>5</sup>       | 2 <sup>3</sup>        | 0.1815        |
| Linear     | 2 <sup>-5</sup>      | -                     | 0.4667        |
| Linear     | 2 <sup>-3</sup>      | -                     | 0.6000        |
| Linear     | 2 <sup>-1</sup>      | -                     | 0.7148        |
| Linear     | 2 <sup>0</sup>       | -                     | 0.8333        |
| Linear     | 2 <sup>1</sup>       | -                     | 0.8407        |
| Linear     | 2 <sup>3</sup>       | -                     | 0.8481        |
| Linear     | 2 <sup>5</sup>       | -                     | 0.8593        |

#### Random Forest (RF)

| Split criteria<br>(criterion) | # of trees<br>(estimators) | The minimum # of<br>samples in a leaf<br>node | Accruacy |
|-------------------------------|----------------------------|---|----------|
|                               |                            | (min samples leaf)                            |          |
| Gini impurity                 | 100                        | 1   | 0.9111   |
| Gini impurity                 | 100                        | 2   | 0.9000   |
| Gini impurity                 | 100                        | 3   | 0.8926   |
| Gini impurity                 | 100                        | 4   | 0.8926   |
| Gini impurity                 | 100                        | 5   | 0.8963   |
| Gini impurity                 | 300                        | 1   | 0.8963   |
| Gini impurity                 | 300                        | 2   | 0.9185   |
| Gini impurity                 | 300                        | 3   | 0.9074   |
| Gini impurity                 | 300                        | 4   | 0.8889   |
| Gini impurity                 | 300                        | 5   | 0.8889   |
| Gini impurity                 | 500                        | 1   | 0.9074   |
| Gini impurity                 | 500                        | 2   | 0.9037   |
| Gini impurity                 | 500                        | 3   | 0.9111   |
| Gini impurity                 | 500                        | 4   | 0.9000   |
| Gini impurity                 | 500                        | 5   | 0.9000   |
| Gini impurity                 | 700                        | 1   | 0.9185   |
| Gini impurity                 | 700                        | 2   | 0.8963   |
| Gini impurity                 | 700                        | 3   | 0.9037   |
| Gini impurity                 | 700                        | 4   | 0.9000   |
| Gini impurity                 | 700                        | 5   | 0.8963   |
| Gini impurity                 | 900                        | 1   | 0.9074   |
| Gini impurity                 | 900                        | 2   | 0.9000   |
| Gini impurity                 | 900                        | 3   | 0.9148   |
| Gini impurity                 | 900                        | 4   | 0.9074   |
| Gini impurity                 | 900                        | 5   | 0.8889   |
| entropy                       | 100                        | 1   | 0.9111   |
| entropy                       | 100                        | 2   | 0.8926   |
| entropy                       | 100                        | 3   | 0.9111   |
| entropy                       | 100                        | 4   | 0.8852   |
| entropy                       | 100                        | 5   | 0.8852   |
| entropy                       | 300                        | 1   | 0.9185   |
| entropy                       | 300                        | 2   | 0.9111   |

|                |            |          |               |
|----------------|------------|----------|---------------|
| <b>entropy</b> | <b>300</b> | <b>3</b> | <b>0.9259</b> |
| entropy        | 300        | 4        | 0.8926        |
| entropy        | 300        | 5        | 0.9037        |
| entropy        | 500        | 1        | 0.9111        |
| entropy        | 500        | 2        | 0.9259        |
| entropy        | 500        | 3        | 0.9074        |
| entropy        | 500        | 4        | 0.9037        |
| entropy        | 500        | 5        | 0.9074        |
| entropy        | 700        | 1        | 0.8963        |
| entropy        | 700        | 2        | 0.9000        |
| entropy        | 700        | 3        | 0.9074        |
| entropy        | 700        | 4        | 0.9074        |
| entropy        | 700        | 5        | 0.8963        |
| entropy        | 900        | 1        | 0.9074        |
| entropy        | 900        | 2        | 0.9037        |
| entropy        | 900        | 3        | 0.9037        |
| entropy        | 900        | 4        | 0.9074        |
| entropy        | 900        | 5        | 0.9000        |

---

**Logistic Regression (LR)**

---

| max_iter<br>(maximum number<br>of iterations to<br>converge) | Penalty parameter (C) | Accuracy      |
|--|-----------------------|---------------|
| 100  | 0.03125               | 0.7185        |
| 100  | 0.125                 | 0.7407        |
| 100  | 0.5                   | 0.7963        |
| 100  | 1                     | 0.7963        |
| 100  | 2                     | 0.8222        |
| <b>100</b>   | <b>8</b>              | <b>0.8259</b> |
| 100  | 32                    | 0.8222        |
| 200  | 0.03125               | 0.7185        |
| 200  | 0.125                 | 0.7407        |
| 200  | 0.5                   | 0.7963        |
| 200  | 1                     | 0.7963        |
| 200  | 2                     | 0.8222        |
| 200  | 8                     | 0.8259        |
| 200  | 32                    | 0.8222        |
| 300  | 0.03125               | 0.7185        |
| 300  | 0.125                 | 0.7407        |
| 300  | 0.5                   | 0.7963        |
| 300  | 1                     | 0.7963        |
| 300  | 2                     | 0.8222        |
| 300  | 8                     | 0.8259        |
| 300  | 32                    | 0.8222        |
| 400  | 0.03125               | 0.7185        |
| 400  | 0.125                 | 0.7407        |
| 400  | 0.5                   | 0.7963        |
| 400  | 1                     | 0.7963        |
| 400  | 2                     | 0.8222        |
| 400  | 8                     | 0.8259        |
| 400  | 32                    | 0.8222        |
| 500  | 0.03125               | 0.7185        |
| 500  | 0.125                 | 0.7407        |
| 500  | 0.5                   | 0.7963        |
| 500  | 1                     | 0.7963        |
| 500  | 2                     | 0.8222        |
| 500  | 8                     | 0.8259        |
| 500  | 32                    | 0.8222        |

---