**Table S1.** Hyperparameters optimised by grid search

|  |  |  |
| --- | --- | --- |
| **Method** | **Parameter** | **Tested values** |
| RF, ERT, and GB | Number of estimators (n\_estimators[a]) | 60–1000 with an interval of 20 |
| Maximum number of features considered per split (max\_features[a]) | 1–20 with an interval of 1, “sqrt[b]”, None[c] |
| Minimum number of samples required to split an internal node (min\_samples\_split[a]) | 2–10 with an interval of 1 |
| SVM | Penalty parameter (C[a]) | [2-15–210] in log2 steps |
| Kernel coefficient ($γ$[a]) | [2-10–210] in log2 steps |
| AB | Maximum number of estimators at which boosting is terminated (n\_estimator[a]) | 20-1000 with an interval of 20. |
| *k*-NN | Number of neighbors (n\_neighbors[a]) | 1-150 with an interval of 1. |

Column 1 represents the ML algorithms. Column 2 and 3 respectively represent the parameter and the tested values. [a] Parameter name in the scikit-learn implementation. [b] default value. [c] all features are used.