

Table 2: A comprehensive overview of common ML models, their hyper-parameters, suitable optimization techniques, and available Python libraries

ML Algorithm	Main HPs	Optional HPs	HPO methods	Libraries
Linear regression	-	-	-	-
Ridge & lasso	alpha	-	BO-GP	Skpot
Logistic regression	penalty, c, solver	-	BO-TPE, SMAC	Hyperopt, SMAC
KNN	n_neighbors	weights, p, algorithm	BOs, Hyperband	Skpot, Hyperopt, SMAC, Hyperband
SVM	C, kernel, epsilon (for SVR)	gamma, coef0, degree	BO-TPE, SMAC, BOHB	Hyperopt, SMAC, BOHB
NB	alpha	-	BO-GP	Skpot
DT	criterion, max_depth, min_samples_split, min_samples_leaf, max_features	splitter, min_weight_fraction_leaf, max_leaf_nodes	GA, PSO, BO-TPE, SMAC, BOHB	TPOT, Optunity, SMAC, BOHB
RF & ET	n_estimators max_depth, criterion, min_samples_split, min_samples_leaf, max_features	splitter, min_weight_fraction_leaf, max_leaf_nodes	GA, PSO, BO-TPE, SMAC, BOHB	TPOT, Optunity, SMAC, BOHB
XGBoost	n_estimators, max_depth, learning_rate, subsample, colsample_bytree,	min_child_weight, gamma, alpha, lambda	GA, PSO, BO-TPE, SMAC, BOHB	TPOT, Optunity, SMAC, BOHB
Voting	estimators, voting	weights	GS	sklearn
Bagging	base_estimator, n_estimators	max_samples, max_features	GS, BOs	sklearn, Skpot, Hyperopt, SMAC
AdaBoost	base_estimator, n_estimators, learning_rate	-	BO-TPE, SMAC	Hyperopt, SMAC
Deep learning	number of hidden layers, units per layer, loss, optimizer, Activation, learning_rate, dropout rate, epochs, batch_size, early stop patience	number of frozen layers (if transfer learning is used)	PSO, BOHB	Optunity, BOHB
K-means	n_clusters	init, n_init, max_iter	BOs, Hyperband	Skpot, Hyperopt, SMAC, Hyperband
Hierarchical clustering	n_clusters, distance_threshold	linkage	BOs, Hyperband	Skpot, Hyperopt, SMAC, Hyperband
DBSCAN	eps, min_samples	-	BO-TPE, SMAC, BOHB	Hyperopt, SMAC, BOHB
Gaussian mixture	n_components	covariance_type, max_iter, tol	BO-GP	Skpot
PCA	n_components	svd_solver	BOs, Hyperband	Skpot, Hyperopt, SMAC, Hyperband
LDA	n_components	solver, shrinkage	BOs, Hyperband	Skpot, Hyperopt, SMAC, Hyperband