

Tunability: Importance of Hyperparameters of Machine Learning Algorithms

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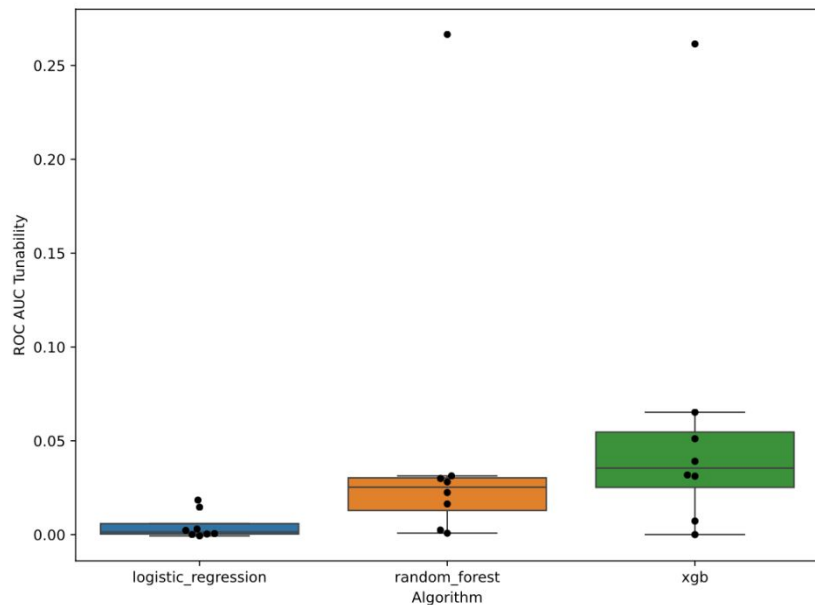
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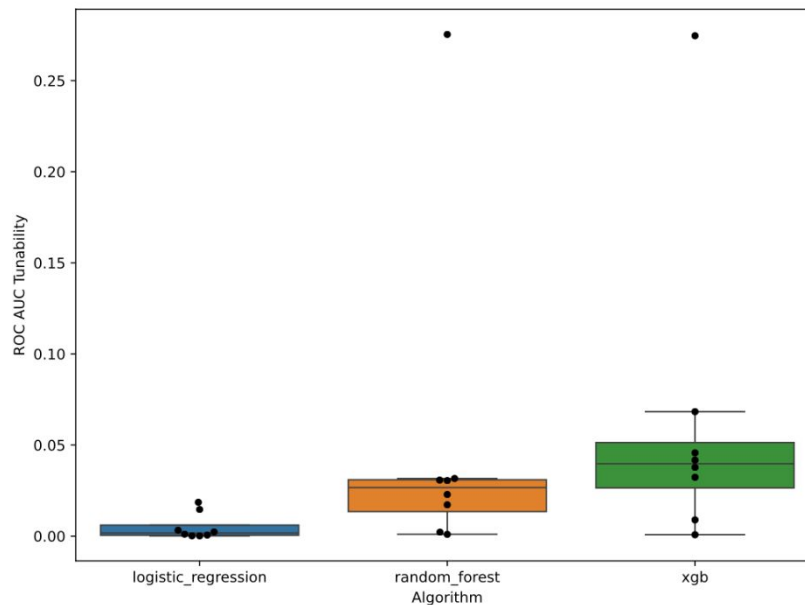
Algorithms & Hyperparameters

Algorithm	Hyperparameter	Lower	Upper	Distribution
logistic regression	C	10^{-3}	10^3	log-uniform
	l1_ratio	0	1	uniform
random forest	n_estimators	10	1000	uniform
	max_depth	1	100	uniform
	min_samples_split	2	10	uniform
	criterion	gini	entropy	–
	min_samples_leaf	1	10	uniform
	max_samples	0.1	1.0	uniform
XGBoost	n_estimators	10	1000	uniform
	max_depth	1	15	uniform
	min_child_weight	1	10	uniform
	subsample	0.1	1.0	uniform
	colsample_bytree	0.1	1.0	uniform
	learning_rate	10^{-3}	1	log-uniform
	reg_alpha	10^{-4}	10^4	log-uniform
	reg_lambda	10^{-4}	10^4	log-uniform

Tunability wrt. package defaults



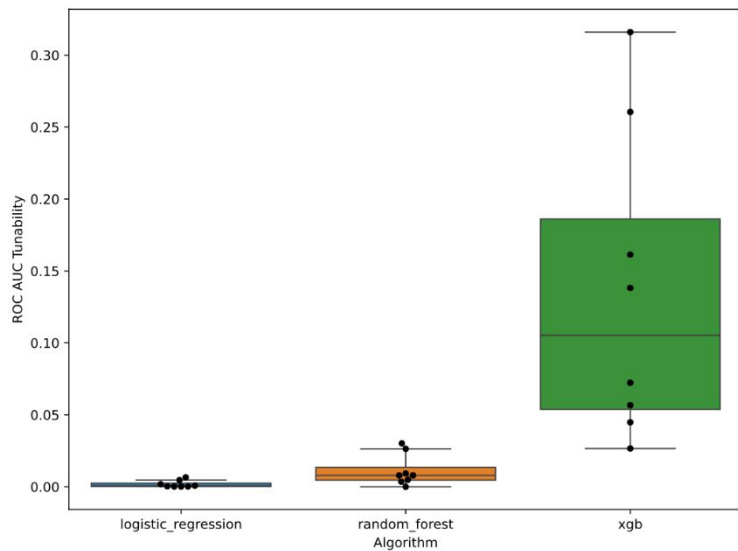
(a) random search



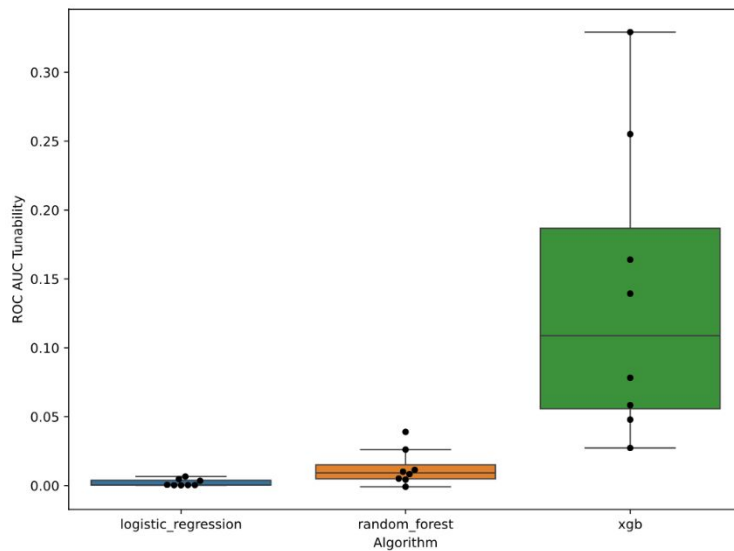
(b) bayesian optimization

Algorithm	Random search tunability	Bayesian search tunability
logistic regression	0.0048 ± 0.0074	0.0051 ± 0.0073
random forest	0.0497 ± 0.0884	0.0514 ± 0.0913
XGBoost	0.0609 ± 0.0838	0.0638 ± 0.0878

Tunability wrt. optimal defaults



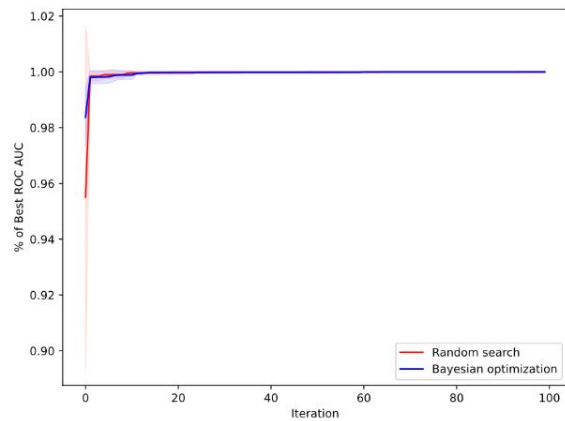
(a) random search



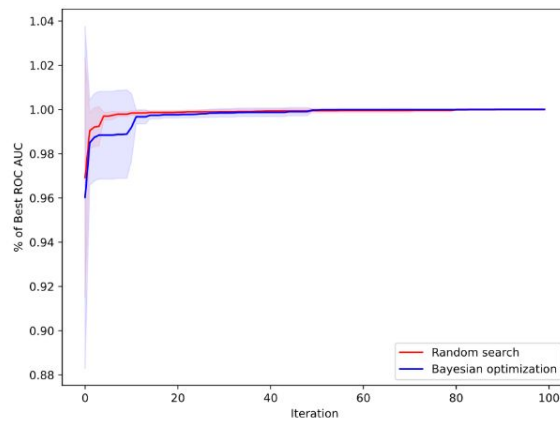
(b) bayesian optimization

Algorithm	Random search tunability	Bayesian search tunability
logistic regression	0.0018 ± 0.0024	0.0021 ± 0.0025
random forest	0.0113 ± 0.0109	0.0129 ± 0.0131
XGBoost	0.1346 ± 0.1064	0.1374 ± 0.1077

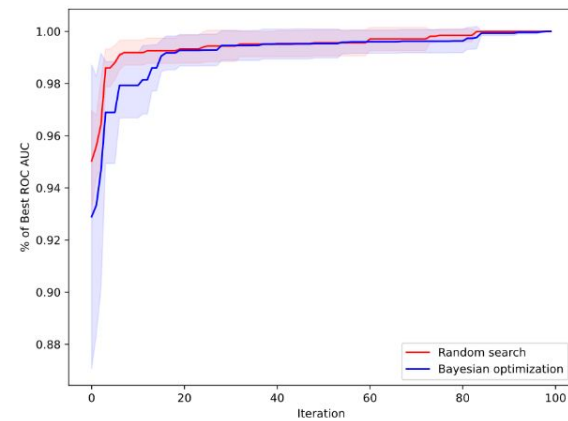
Optimization dynamics



(a) logistic regression



(b) random forest



(c) XGBoost