

Random forest parameter tuning

For the parameter optimisation results we present in the main test we run a nested cross-validation experiment over a grid spanning 6 parameters and a total of 96 points. We chose these parameters to include following the description in the documentation of scikit-learn documentation (<https://scikit-learn.org/stable/modules/ensemble.html>). The 6 parameters together with their default value (in brackets) and their alternative values are listed below:

- 'bootstrap': [True], False
- 'max_depth': [None], 10
- 'max_features': ['auto'], 'sqrt'
- 'min_samples_leaf': [1], 2
- 'min_samples_split': [2], 4
- 'n_estimators': [100], 25, 200

In Table A we list the MSE (average, minimum and maximum over the 10 splits) obtained from the nested cross-validation optimisation run for the 96 points of the parameters grid. We also list the rank (average, minimum and maximum over the 10 splits) in terms of the achieved MSE for each grid point. For the 'bootstrap' and 'max_features' parameters for which the 'TRUE' and 'sqrt' values are performing consistently better. For the other 4 parameters there does not seem to be a clear separation between better and worse performing values.

Table A: MSE performance and rank of the 96 parameter sets in the double-loop nested cross-validation experiment. The default parameter setup is in bold font.

boots trap	max_depth	max_features	min_samples_leaf	min_samples_split	n_estimators	Mean MSE OverSplits	Min MSE OverSplits	Max MSE OverSplits	Mean Rank OverSplits	MinRankOverSplits	MaxRankOverSplits
TRUE	10	sqrt	2	2	200	8.41	8.13	8.70	4.5	1	11
TRUE	10	sqrt	2	4	200	8.41	8.13	8.70	4.5	1	11
TRUE	None	sqrt	2	2	200	8.41	8.13	8.73	4.6	1	9
TRUE	None	sqrt	2	4	200	8.41	8.13	8.73	4.6	1	9
TRUE	None	sqrt	2	2	100	8.46	8.10	8.76	6	1	11
TRUE	None	sqrt	2	4	100	8.46	8.10	8.76	6	1	11
TRUE	10	sqrt	2	2	100	8.46	8.10	8.75	7.5	3	12
TRUE	10	sqrt	2	4	100	8.46	8.10	8.75	7.5	3	12
TRUE	None	sqrt	2	2	25	8.58	8.05	9.01	11.3	1	33
TRUE	None	sqrt	2	4	25	8.58	8.05	9.01	11.3	1	33
TRUE	10	sqrt	2	2	25	8.60	8.05	8.92	12.1	1	30
TRUE	10	sqrt	2	4	25	8.60	8.05	8.92	12.1	1	30
TRUE	None	sqrt	1	4	200	8.78	8.43	9.14	16.1	9	26
TRUE	10	sqrt	1	4	200	8.78	8.46	9.16	17.2	9	28
TRUE	None	sqrt	1	4	100	8.81	8.53	9.36	17.3	13	25
TRUE	10	sqrt	1	4	100	8.80	8.53	9.37	17.9	10	28
TRUE	10	auto	2	2	200	8.99	8.41	9.64	22.5	13	33
TRUE	10	auto	2	4	200	8.99	8.41	9.64	22.5	13	33
TRUE	None	auto	2	2	200	8.99	8.41	9.64	22.9	15	31
TRUE	None	auto	2	4	200	8.99	8.41	9.64	22.9	15	31
TRUE	10	auto	2	2	100	9.04	8.52	9.84	23.7	11	37
TRUE	10	auto	2	4	100	9.04	8.52	9.84	23.7	11	37
TRUE	None	auto	2	2	100	9.04	8.54	9.85	24.4	13	37
TRUE	None	auto	2	4	100	9.04	8.54	9.85	24.4	13	37
TRUE	10	sqrt	1	4	25	9.03	8.47	9.61	25.7	9	48
TRUE	None	sqrt	1	4	25	9.02	8.49	9.63	26.3	14	50
TRUE	None	sqrt	1	2	200	9.09	8.62	9.67	27	17	36
TRUE	10	sqrt	1	2	200	9.11	8.60	9.70	27.6	14	37
TRUE	None	sqrt	1	2	100	9.12	8.62	9.85	28	16	37
TRUE	10	sqrt	1	2	100	9.15	8.64	9.94	28.4	10	38
TRUE	None	auto	2	2	25	9.28	8.69	10.51	34.3	3	59
TRUE	None	auto	2	4	25	9.28	8.69	10.51	34.3	3	59
TRUE	10	auto	2	2	25	9.28	8.65	10.49	34.6	1	55
TRUE	10	auto	2	4	25	9.28	8.65	10.49	34.6	1	55
TRUE	10	sqrt	1	2	25	9.35	8.47	10.23	36.3	14	47
TRUE	None	sqrt	1	2	25	9.36	8.29	10.27	37	13	58
TRUE	10	auto	1	4	100	9.54	8.63	10.61	41	18	54
TRUE	None	auto	1	4	100	9.54	8.66	10.60	41.4	23	53
TRUE	10	auto	1	4	25	9.64	8.55	11.55	41.8	15	68

TRUE	None	auto	1	4	200	9.55	8.74	10.37	41.8	15	55
TRUE	None	auto	1	4	25	9.63	8.60	11.53	41.9	22	67
TRUE	10	auto	1	4	200	9.55	8.77	10.39	42	16	56
FALSE	None	sqrt	2	2	100	9.57	9.11	10.27	43.9	27	54
FALSE	None	sqrt	2	4	100	9.57	9.11	10.27	43.9	27	54
FALSE	10	sqrt	2	2	100	9.57	9.11	10.16	44.1	25	55
FALSE	10	sqrt	2	4	100	9.57	9.11	10.16	44.1	25	55
FALSE	None	sqrt	2	2	200	9.62	9.10	10.33	45.4	31	59
FALSE	None	sqrt	2	4	200	9.62	9.10	10.33	45.4	31	59
FALSE	10	sqrt	2	2	200	9.61	9.11	10.19	45.5	29	60
FALSE	10	sqrt	2	4	200	9.61	9.11	10.19	45.5	29	60
FALSE	10	sqrt	2	2	25	9.63	9.22	10.13	47.3	21	62
FALSE	10	sqrt	2	4	25	9.63	9.22	10.13	47.3	21	62
FALSE	None	sqrt	2	2	25	9.66	9.02	10.10	47.8	27	65
FALSE	None	sqrt	2	4	25	9.66	9.02	10.10	47.8	27	65
TRUE	None	auto	1	2	200	9.85	8.87	10.73	50.5	27	60
TRUE	10	auto	1	2	200	9.85	8.92	10.76	50.7	32	60
TRUE	10	auto	1	2	100	9.85	9.00	11.01	51.1	36	60
TRUE	None	auto	1	2	100	9.87	8.95	11.11	51.4	35	61
TRUE	None	auto	1	2	25	10.00	8.87	12.13	52	38	72
TRUE	10	auto	1	2	25	9.98	8.91	11.79	52.2	40	71
FALSE	None	sqrt	1	4	100	10.41	9.18	11.67	59.5	49	64
FALSE	None	sqrt	1	4	200	10.42	9.21	11.58	60.1	51	64
FALSE	10	sqrt	1	4	200	10.44	9.25	11.46	60.6	52	66
FALSE	10	sqrt	1	4	100	10.46	9.27	11.53	61.1	53	67
FALSE	None	sqrt	1	4	25	10.65	9.40	11.75	62.9	59	66
FALSE	10	sqrt	1	4	25	10.78	9.46	12.21	64.3	61	66
FALSE	None	sqrt	1	2	100	11.18	9.84	12.58	69.3	64	82
FALSE	None	sqrt	1	2	200	11.22	9.79	12.62	69.5	63	83
FALSE	10	sqrt	1	2	200	11.22	9.76	12.66	69.6	65	81
FALSE	10	sqrt	1	2	100	11.22	9.81	12.87	69.8	66	80
FALSE	None	sqrt	1	2	25	11.46	9.99	13.04	71.8	67	84
FALSE	10	sqrt	1	2	25	11.46	9.84	13.27	72.7	65	84
FALSE	10	auto	2	2	25	13.16	11.36	18.22	80.8	71	91
FALSE	10	auto	2	4	25	13.16	11.36	18.22	80.8	71	91
FALSE	None	auto	2	2	25	13.14	11.42	18.00	80.8	71	93
FALSE	None	auto	2	2	100	13.18	11.38	18.27	80.8	73	89
FALSE	None	auto	2	4	25	13.14	11.42	18.00	80.8	71	93
FALSE	None	auto	2	4	100	13.18	11.38	18.27	80.8	73	89
FALSE	10	auto	2	2	100	13.18	11.29	18.32	81.4	73	95
FALSE	10	auto	2	4	100	13.18	11.29	18.32	81.4	73	95
FALSE	10	auto	2	2	200	13.19	11.24	18.41	81.6	67	95
FALSE	10	auto	2	4	200	13.19	11.24	18.41	81.6	67	95
FALSE	None	auto	2	2	200	13.19	11.30	18.42	81.6	69	95

FALSE	None	auto	2	4	200	13.19	11.30	18.42	81.6	69	95
FALSE	10	auto	1	4	25	14.99	10.81	19.30	81.8	73	90
FALSE	None	auto	1	4	25	14.97	10.65	19.06	82.7	73	89
FALSE	None	auto	1	4	200	15.02	10.61	19.07	83.6	73	89
FALSE	10	auto	1	4	200	15.05	10.71	19.24	83.8	76	90
FALSE	10	auto	1	4	100	15.07	10.69	19.27	84	76	90
FALSE	None	auto	1	4	100	15.03	10.62	19.05	84.1	74	90
FALSE	10	auto	1	2	25	16.23	11.16	21.21	89.1	80	96
FALSE	None	auto	1	2	25	16.26	11.22	21.05	89.3	79	96
FALSE	None	auto	1	2	200	16.27	11.10	21.17	89.8	79	95
FALSE	None	auto	1	2	100	16.29	11.10	21.18	90.1	79	96
FALSE	10	auto	1	2	200	16.31	11.22	21.38	90.2	81	96
FALSE	10	auto	1	2	100	16.33	11.25	21.43	90.9	83	96