Author: Echtenbruck, M.M.
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Appendices

Appendix A

Supplementary Results

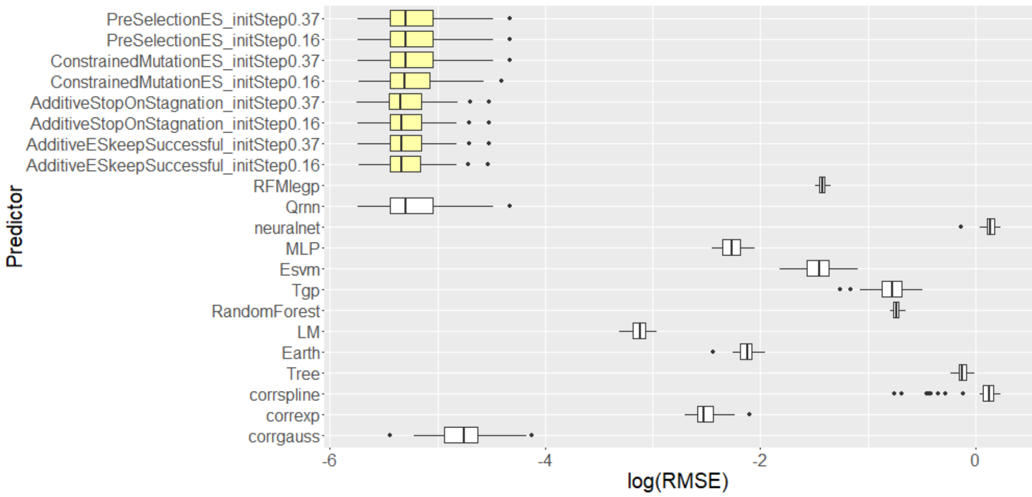
A large number of experiments was carried out for this thesis, and an even larger number of result plots was generated for the evaluation of these experiments. For the sake of readability, only the most relevant plots were shown in the main part of this thesis. In the following, supplementary plots are provided that also may be of interest since they provide further insights into the functionality and performance of the proposed ensemble method.

A.1 N-ary Ensembles on Higher Dimensional Physical Functions

In Section 4.5 experiments were carried out to compare the ensemble building method using different adaptations of the ES to each other and all base models. The results presented were condensed to the relevant information, each time showing only the results of the best performing base model, to preserve the readability. For the sake of completeness and to prove that no important information was omitted, in the following, the results for all base models are presented.

Figure A.1 shows the results for the experiments on the otl-circuit function (cf. Figure A.1a) and on the piston function (cf. Figure A.1b). On these functions, the ensemble adaptations and the best base model show comparable results and perform significantly better than the remaining base models, whose performances are heavily varying.

(a) Result on the otl-circuit function.



(b) Result on the piston function.

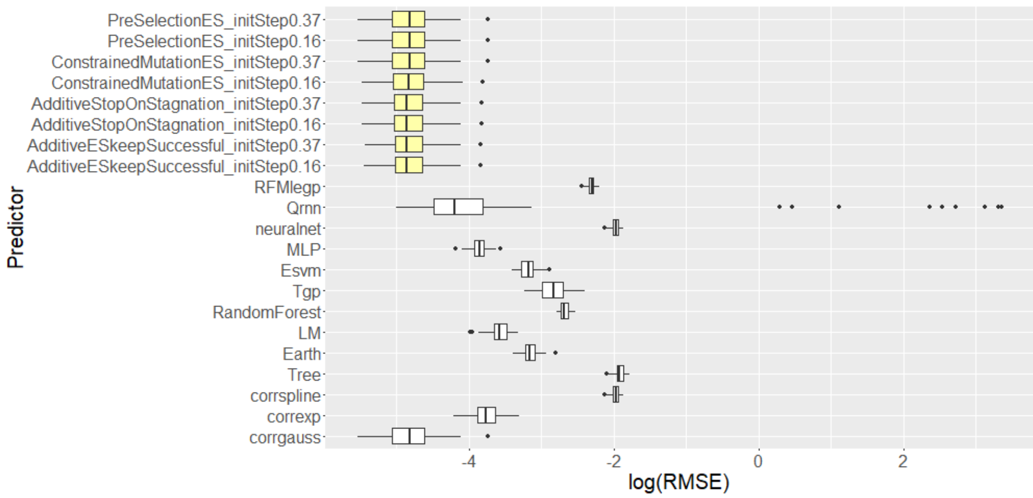
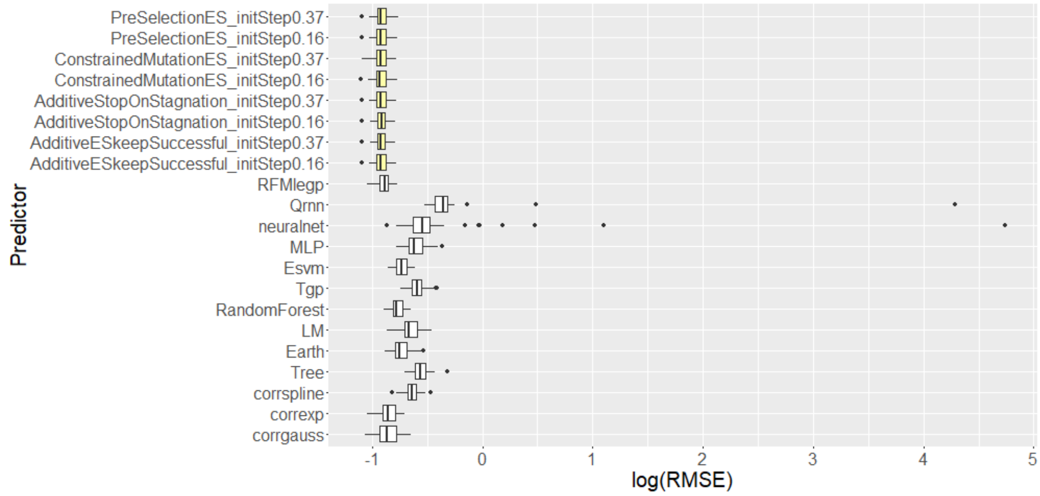


Figure A.1: The plot shows the results of the comparison of the performances, in terms of RMSE, of the different adaptations of the ensemble building method and all base models on the otl-circuit function and the piston function. Ensemble results are colored yellow, the base model result is shown in white. The ensemble adaptations can compete with the best base model and perform clearly better than all remaining base models.

(a) Result on the robot function. The ensemble adaptations can compete with the best base model. Correxp and Corrgauss also show comparable performances, only slightly weaker than the best base model and the ensemble adaptations. All remaining base models perform significantly worse.



(b) Result on the wing weight function. The ensemble adaptations belong to the better performing models.

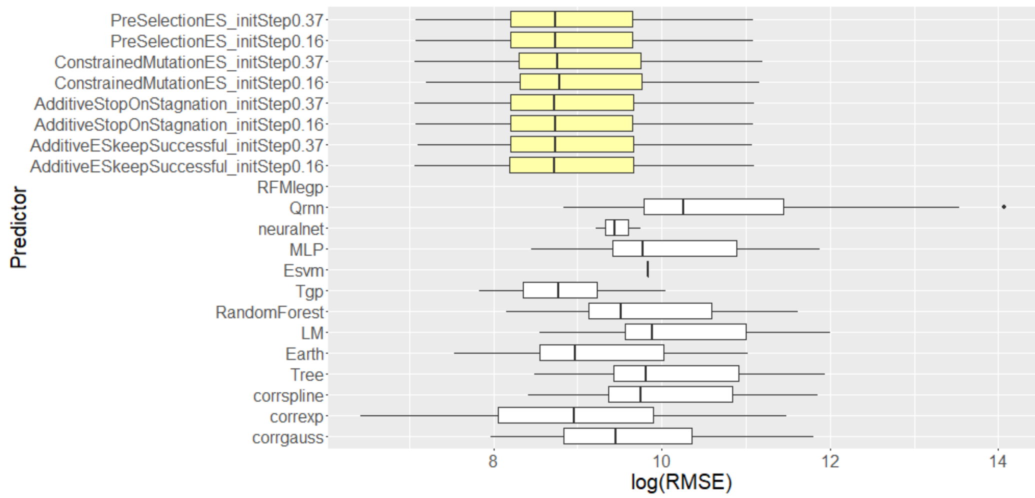


Figure A.2: The plot shows the results of the comparison of the performances, in terms of RMSE, of the different adaptations of the ensemble building method and all base models on the robot function and the wing weight function. Ensemble results are colored yellow, the base model result is shown in white.

Remarkable is that despite the large variance in the performances of the base models, the ensembles show a steady performance with a standard deviation comparable to or even slightly better than the one of the best base model.

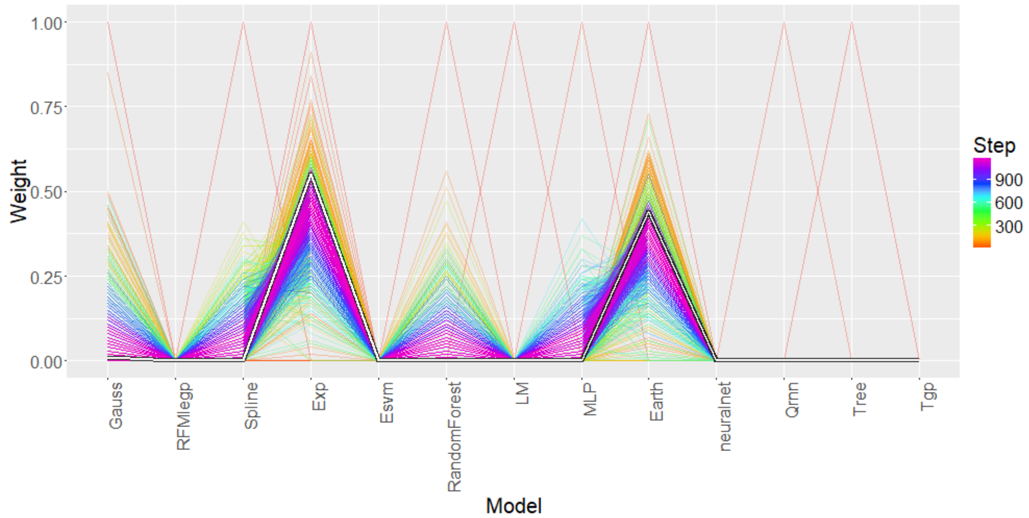
Figure A.2 shows the results for the experiments on the robot function (cf. Figure A.2a) and on the wing weight function (cf. Figure A.2b).
On the robot function, the ensembles and the best base model again show comparable performance. The base models ranked second and third, corrgauss and correxp, already perform slightly worse and all remaining base models perform significantly worse than the ensemble adaptations. Like on the otl-circuit function and the piston function this variance in the performances of the base models does not influence the good performance of the ensemble.
On the wing weight function, the results are more close; only one base model performs significantly worse than all ensemble adaptations. Still, the ensembles are among the best performing models.

In the following, a closer look is taken at the behavior of the different ensemble approaches. Exemplary plots are shown for the optimization of the weights to find the best model on the otl-circuit function (cf. Figures A.3 and A.4). The plots document the development of the weights for each step of the search. Each line represents a single individual considered during the search, and its color marks the related search step when the individual was found.

In all of these plots can be seen, that the base models RFMlegp, Esvm, neuralnet and Tgp did not receive any weight throughout the whole search. This is owed to the fact that these models failed during the preceding cross-evaluation in at least one, but rather most or even all of the evaluations. To obtain a reliable ensemble, models that failed in at least one of the evaluation steps are excluded from the search for the best weights.

Figure A.3 shows the development of the weights during the optimization using the additive approaches. The characteristics of these approaches can be easily read from the plots. The additive approach, which stops after the search stagnates (cf. Figure A.3a), ends the search after the addition of MLP. Previously added base models at least gained small weight during the search, but no improvement could be made with the addition of MLP. As a result, the search stopped.
The additive approach that does not stop on stagnation considered all base models. The course of the optimization can be read from the plot (cf. Figure A.3b). The three base models Gauss, Exp and Earth that were part of the search space from the start on, show nearly the complete range of colors.

(a) Sequential addition with stop on stagnation. After the search stagnates with the addition of MLP the search is stopped. Therefore, the base models LM, Qrnn and tree that are ranked lower than MLP are not considered in this search.



(b) Sequential addition without stop on stagnation. All base models are considered.

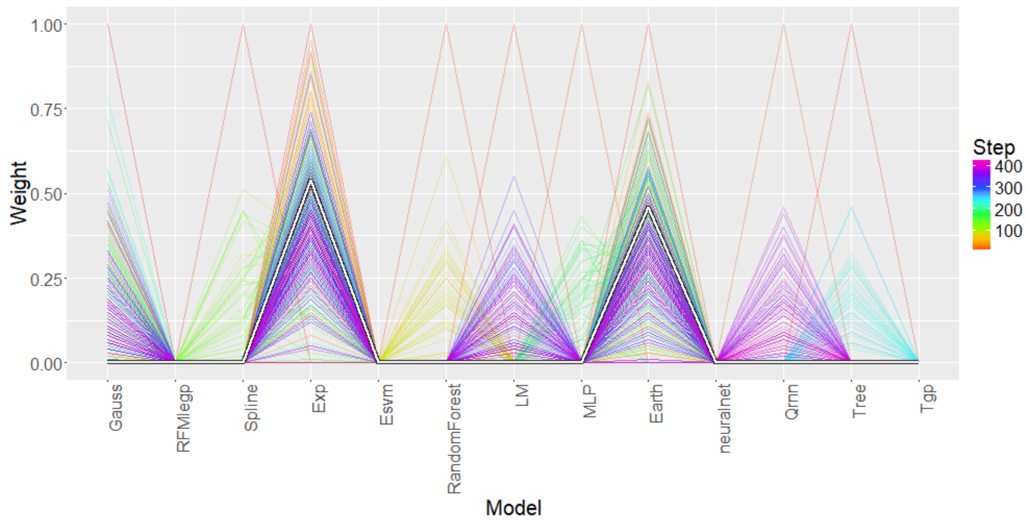
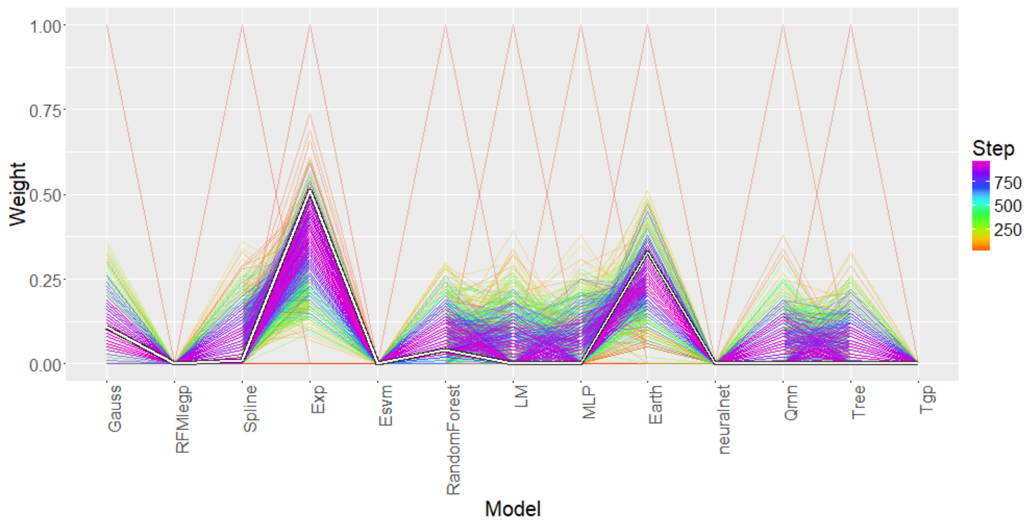


Figure A.3: The plots document the development of the weights during the optimization for the otl-circuit function using the additive approaches. Each line represents a single individual considered during the search, and its color marks the related search step when the individual was found, the white line marks the best weights combination. Though, through the course of the optimization both approaches consider different individuals, in the end, they agree on similar weight combinations.

(a) Restriction of the mutation.



(b) Preselection of models. During the automatized preselection of the base models, the search space is restricted to the three best-ranked base models.

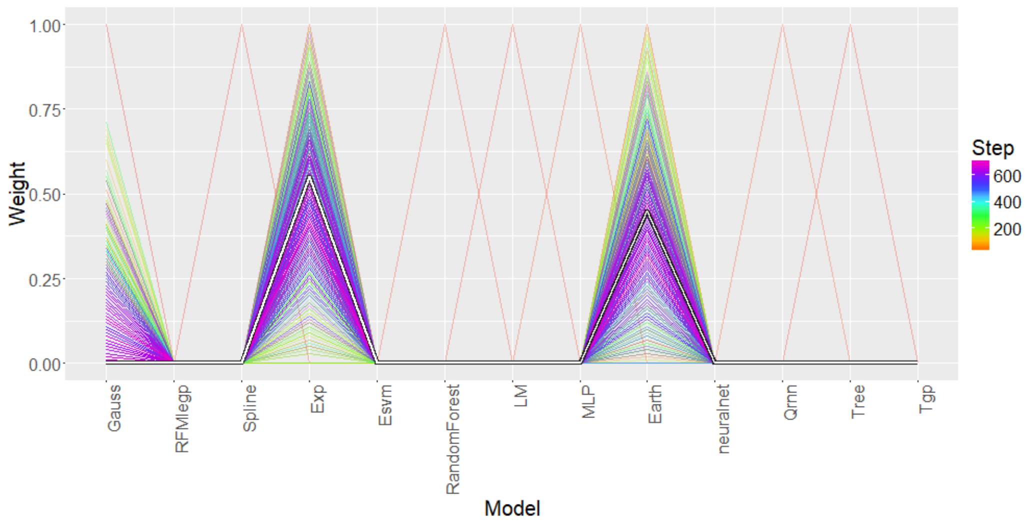


Figure A.4: The plots document the development of the weights during the optimization for the otl-circuit function using the approaches that restrict the search space and the mutation respectively. Each line represents a single individual considered during the search, and its color marks the related search step when the individual was found, the white line marks the best weights combination.

The base models that were added later in the course of the optimization show only a limited range of colors.
In the end, both approaches agree on similar best weights for the best ensemble combination.

Figure A.4 shows the development of the weights during the optimization using the approaches that restrict the considered base models or the mutation respectively. Again, the characteristics of these approaches can be easily read from the plots.
The approach that restricts the mutation searches the complete search space throughout the course of the optimization. No structure in the search can be read from the plot; the course of the search seems random. The final search result visibly differs from the weight combinations preferred by the additive approaches although most weight is given to the same base models.
The approach that initially selects a subset of the available base models for optimization using a rule based on the comparison to the mean predictor as described in Section 4.4.4. Applying this rule, the search is restricted to the base models Gauss, Exp, and Earth. The search on these base models again leads to similar weights as already preferred by the additive approaches.

A.2 The Performance of Dynamical Adapted CCM in SPO

In Section 5.2.5 the CCMs using $\tau = 1, \lambda = 10$ and $\tau = 20, \lambda = 20$ respectively were compared to two strong ensemble competitors and all base models. The results presented were condensed to the relevant information to preserve the readability. For the sake of completeness, in the following, the complete results for all base models are given and discussed.

Table A.1 presents these results. Given are the mean and standard deviation for the results of the optimization processes, best results are marked bold. To allow for a comparison of the models over the different functions, the mean results are function-wise ranked, and the average ranking, as well as the final rank for each model, is given in the two last rows.
Some of the entries show a red 'N/A'. These entries refer to experimental setups where the optimization process using the stated model did not succeed in at least one repetition. Therefore, the related rankings in the two last rows are given in brackets.

	$\tau=1,\lambda=10$	correxp	corrgauss	corrspline	Earth	Lm
ackley2D	2.4957 (±1.931)	7.6620 (±1.465)	2.1552 (±3.055)	3.2729 (±3.189)	5.8966 (±1.853)	3.1309 (±1.741)
ackley4D	6.8503 (±3.179)	11.588 (±1.275)	5.3801 (±3.576)	7.8778 (±4.558)	8.1570 (±1.870)	**5.2055** (±1.074)
GLG4D	22.430 (±12.00)	33.021 (±5.766)	**21.101** (±13.17)	26.344 (±10.49)	29.465 (±10.19)	32.479 (±9.483)
GLG8D	29.616 (±9.420)	57.321 (±7.660)	**28.702** (±11.39)	42.634 (±20.82)	60.226 (±4.488)	56.429 (±6.917)
otl-circuit	2.6055 (±0.002)	2.6542 (±0.034)	2.6553 (±0.070)	2.7007 (±0.070)	**2.6039** (±0.000)	N/A
piston	**0.1667** (±0.003)	0.1708 (±0.002)	0.1709 (±0.005)	0.1750 (±0.011)	0.1670 (±0.001)	0.1761 (±0.011)
robot	0.0132 (±0.020)	0.0552 (±0.027)	0.0309 (±0.015)	0.0756 (±0.044)	0.0253 (±0.022)	0.0169 (±0.036)
rosenbrock4D	**2.4138** (±1.522)	288.78 (±300.4)	3.5536 (±2.490)	60.989 (±138.8)	727.23 (±610.5)	70.933 (±63.79)
rosenbrock8D	4127.1 (±2989)	3188.6 (±1474)	6819.3 (±2799)	18887 (±12949)	23688 (±12099)	**696.83** (±582.0)
wingweight	182.50 (±13.11)	174.83 (±14.12)	178.91 (±14.44)	181.05 (±6.350)	175.94 (±6.323)	185.10 (±12.82)
AVG RANK	3.6	7.2	4.2	6.95	7.05	(5.7)
RANK	2	11	3	7	10	(5)

	$\tau=20,\lambda=20$	MLP	Neuralnet	RandomForest	Tgp	tree
ackley2D	1.9344 (±2.041)	**0.3425** (±0.694)	7.8315 (±2.263)	2.5598 (±1.198)	1.1200 (±0.522)	5.6125 (±1.443)
ackley4D	6.0215 (±3.242)	9.7943 (±3.098)	15.330 (±2.523)	8.9207 (±1.946)	5.8991 (±1.028)	15.540 (±0.936)
GLG4D	23.576 (±13.02)	25.799 (±10.63)	33.676 (±9.031)	30.801 (±7.160)	21.690 (±12.28)	32.181 (±8.249)
GLG8D	30.335 (±7.166)	48.353 (±7.637)	56.281 (±1.467)	53.407 (±6.857)	59.229 (±6.998)	58.156 (±6.744)
otl-circuit	2.6103 (±0.012)	**2.6039** (±0.000)	2.8980 (±0.191)	2.7849 (±0.116)	2.7580 (±0.045)	3.0001 (±0.092)
piston	0.1704 (±0.008)	0.1669 (±0.001)	0.2107 (±0.014)	0.1706 (±0.003)	0.1770 (±0.002)	0.2027 (±0.016)
robot	0.0181 (±0.018)	**0.0000** (±0.000)	**0.000** (±0.000)	0.0239 (±0.033)	0.06681 (±0.032)	0.0876 (±0.056)
rosenbrock4D	4.1977 (±2.088)	815.76 (±560.3)	N/A	253.76 (±212.2)	306.48 (±222.6)	732.86 (±689.9)
rosenbrock8D	3224.2 (±2041)	17994 (±12828)	N/A	4705.0 (±2657)	6633.4 (±3569)	23605 (±15191)
wingweight	**173.0** (±10.35)	181.99 (±11.02)	N/A	184.59 (±12.15)	182.94 (±9.371)	181.05 (±12.88)
AVG RANK	**3.4**	5.2	(6.65)	7	7	10
RANK	**1**	4	(6)	8.5	8.5	12

Table A.1: The table displays the results for the main experiment setup. Given are mean optimization result with standard deviation for the CCMs in comparison to all base models.

The most important result here is that the two CCMs are ranked first and second, unlike before, where the CCMs were ranked second and third only. This is owed to the fact, that in the previous representation for each function only the best performing base model was considered, and this best base model, though changing for each function, ranked as one in the overall ranking.
Noteworthy are also the results for the rosenbrock functions. The optimization results obtained from the different base models and the two ensembles range between 2.4 and 816 for rosenbrock4D and between 697 and 23688 for rosenbrock 8D. Though the variance in the performances of the different base models is large, the ensembles showed good performances on both functions; the CCM using $\tau = 1, \lambda = 10$ even performed best on the rosenbrock4D function.

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Glossary

Abbreviations

AIC	Akaike's Information Criterion	37
CCM	Convex Combinations of Models	52
CFD	Computational Fluid Dynamics	3
DOE	Design of Experiment	25
ES	Evolutionary Strategy	64
GMSE	Generalized Mean Squared Error	45
MARS	Multivariate Adaptive Regression Splines	19
MSE	Mean Squared Error	45
RMSE	Root Mean Squared Error	45
SBO	Surrogate Based Optimization	6
SPO	Sequential Parameter Optimization	4
SPOT	Sequential Parameter Optimization Toolbox	4
SVM	Support Vector Machine	17
wRMSE	Weighted Root Mean Squared Error	90

Variables and Identifiers

$\alpha,\ (1-\alpha)$	The Weights Used for the Binary Model Definition	52

α, β, γ	The Weights for the Convex Combination of Models	61
$\hat{y}$	The Predicted Function Value	9
$\mathbf{av}$	A vector of flags, indicating active and suspended models	93
σ	The Step Width of the (1+1)-ES	64
σ_{init}	The Initial Step Width of the (1+1)-ES	64
σ_{min}	Minimum step size of the (1+1)-ES	99
τ	Ensemble Building Interval	88
C	Candidate set for evaluation on the objective function in each sequential step, , with respect to exploration or exploitation respectively (cf. Chapter 2.2)	27
D	Observed Data	25
d	The Dimension	61
M	The Surrogate Model	26
M^*	The Fitted Surrogate Model	26
P	The population of the (1+1)-ES	93
y	The Observed Function Value	9
ρ	Density of the Immediate Neighborhood of a Point	90
$n_{\mathbf{eval}}$	Function Evaluations per Sequential Step	26