Benchmarking Energy Quantification Methods to Predict Heating Energy Performance of Residential Buildings in Germany

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Appendix (available online via http://link.springer.com)

A1 Hyperparameter tuning

Table A 1 Tuned hyperparameter set for the best-performing Artificial Neural Network from the nested cross-validation. The superscript * implies that after mutation no bound was applied

Hyperparameter	**Number of layers**	**Neurons per layer**	**Dropout rate**	**Learning rate**	**Batch-size**
Ranges	$[1, 50]$	$[5, 200]$	$[0, 0.95]$	$[10^{-7}, 10^{0}]$	$[2^{2}, 2^{10}]$
Tuned values	1	69	0	$10^{-2.64}$	2^{2}

Table A 2 Tuned hyperparameter set for the best-performing Extreme Gradient Boosting from the nested cross-validation. The superscript * implies that after mutation no bound was applied

Hyperparameter	**Eta**	**Gamma**	**Maximum depth**	**Minimum child weight**
Ranges	$[10^{-3}, 10^{-0.3}]$	$[0, 5^{*}]$	$[1, 10]$	$[0, 5^{*}]$
Tuned values	$10^{-1.18}$	2.38	4	3.38
Hyperparameter	**Column-sample**	**Sub-sample**	**Alpha**	**Lambda**
Ranges	$[0.05, 1]$	$[0.05, 1]$	$[0, 5^{*}]$	$[0, 5^{*}]$
Tuned values	0.80	0.65	3.20	6.83

Table A 3 Tuned hyperparameter set for the best-performing Random Forest from the nested cross-validation. The superscript * implies that after mutation no bound was applied

Hyperparameter	**Minimum node size**	**Maximum number of leaves**	**Random elements**	**Number of trees**
Ranges	$[2^{0}, 2^{7*}]$	$[2^{-3},\ 2^{5*}]$	$[1, 14]$	$[2^{4}, 2^{10}]$
Tuned values	$2^{1.7}$	$2^{7.8}$	6	2^{9}

Table A 4 Tuned hyperparameter set for the best-performing Support Vector Regression from the nested cross-validation. The superscript * implies that after mutation no bound was applied

Hyperparameter	**Cost**	**Epsilon**	**Gamma**
Ranges	$[2^{-4}, 2^{4}]$	$[0, 2]$	$[2^{-6}, 2^{-3}]$
Tuned values	$2^{-0.72}$	0.86	$2^{-4.78}$

A2 Copula Structure

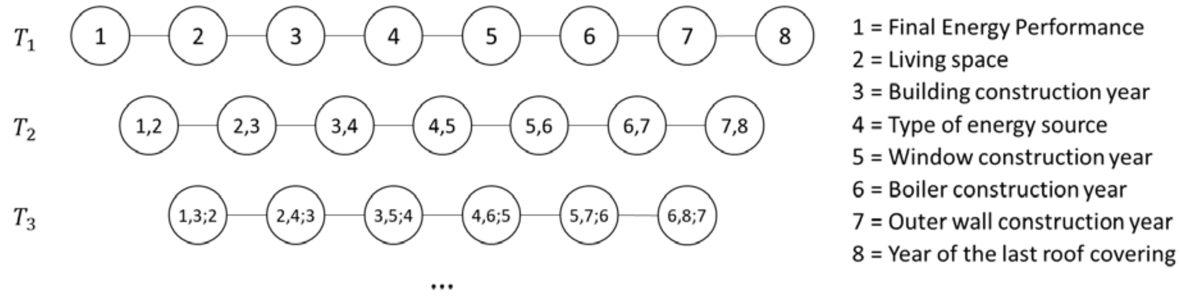

Figure A 1 Resulting D-vine copula structure.
The sequences indicate the trees, the higher-order trees follow analogously

A3 Supervised Machine Learning Reportcard

Table A 5 Supervised Machine Learning Reportcard for rigour documentation following the design by Kühl et al. (2020)

<table>
<tr><th rowspan="6">General Information</th><th>Problem statement</th><td colspan="3">Predict Final Energy Performance of single- and two-family houses in Germany with multiple attributes/variables</td></tr>
<tr><th>Data gathering</th><td colspan="3">The data originates from the nationwide “Modernisierungs-Kompass” (Modernization Compass) offered by the EN-OP Institute (enop.de) as well as from two German energy consultant companies (c.f. Section 4)</td></tr>
<tr><th>Sampling</th><td colspan="3">No sampling of data (post-stratification for Performance Evaluation Measures)</td></tr>
<tr><th>Data quality</th><td colspan="3">Generally high, partly missing or incorrect values</td></tr>
<tr><th>Data pre-processing methods</th><td colspan="3">c.f. Section 4</td></tr>
<tr><th>Feature engineering and vectorizing</th><td colspan="3">c.f. Section 4</td></tr>
<tr><th rowspan="2">All</th><th>Performance evaluation measure for hyperparameter tuning</th><td colspan="3">Stratified Coefficient of Variation, stratification according to German building stock</td></tr>
<tr><th>Parameters</th><td colspan="3">c.f. Appendix A1</td></tr>
<tr><th rowspan="5">ANN</th><th rowspan="2">Parameter optimization</th><td rowspan="2">Yes</td><th>Search space</th><td>c.f. Appendix A1</td></tr>
<tr><th>Search algorithm</th><td>Genetic algorithms</td></tr>
<tr><th>Data split</th><td colspan="3">Nested cross-validation, 5 outer folds, 10 inner folds</td></tr>
<tr><th>Performance evaluation measure for training</th><td colspan="3">Mean Squared Error</td></tr>
<tr><th>Performance measure increase between test and train (risk of overfitting)</th><td colspan="3">1.86 % (stratified Coefficient of Variation)</td></tr>
<tr><th rowspan="4">Copula</th><th>Parameter optimization</th><td colspan="3">No (no hyperparameter)
Nonparametric bivariate building blocks, parsimonious forward selection, AIC as termination criterion</td></tr>
<tr><th>Data split</th><td colspan="3">10-fold cross-validation</td></tr>
<tr><th>Performance evaluation measure for training</th><td colspan="3">Conditional loglikelihood</td></tr>
<tr><th>Performance measure increase between test and train (risk of overfitting)</th><td colspan="3">0.13 % (stratified Coefficient of Variation)</td></tr>
<tr><th rowspan="5">XGB</th><th rowspan="2">Parameter optimization</th><td rowspan="2">Yes</td><th>Search space</th><td>c.f. Appendix A1</td></tr>
<tr><th>Search algorithm</th><td>Genetic algorithms</td></tr>
<tr><th>Data split</th><td colspan="3">Nested cross-validation, 5 outer folds, 10 inner folds</td></tr>
<tr><th>Performance evaluation measure for training</th><td colspan="3">Mean Squared Error</td></tr>
<tr><th>Performance measure increase between test and train (risk of overfitting)</th><td colspan="3">3.44 % (stratified Coefficient of Variation)</td></tr>
<tr><th rowspan="5">RF</th><th rowspan="2">Parameter optimization</th><td rowspan="2">Yes</td><th>Search space</th><td>c.f. Appendix A1</td></tr>
<tr><th>Search algorithm</th><td>Genetic algorithms</td></tr>
<tr><th>Data split</th><td colspan="3">Nested cross-validation, 5 outer folds, 10 inner folds</td></tr>
<tr><th>Performance evaluation measure for training</th><td colspan="3">Mean Squared Error</td></tr>
<tr><th>Performance measure increase between test and train (risk of overfitting)</th><td colspan="3">9.35 % (stratified Coefficient of Variation)</td></tr>
<tr><th rowspan="5">SVR</th><th rowspan="2">Parameter optimization</th><td rowspan="2">Yes</td><th>Search space</th><td>c.f. Appendix A1</td></tr>
<tr><th>Search algorithm</th><td>Genetic algorithms</td></tr>
<tr><th>Data split</th><td colspan="3">Nested cross-validation, 5 outer folds, 10 inner folds</td></tr>
<tr><th>Performance evaluation measure for training</th><td colspan="3">Support Vector Regression objective function</td></tr>
<tr><th>Performance measure increase between test and train (risk of overfitting)</th><td colspan="3">1.80 % (stratified Coefficient of Variation)</td></tr>
</table>

A4 Variable importance plot

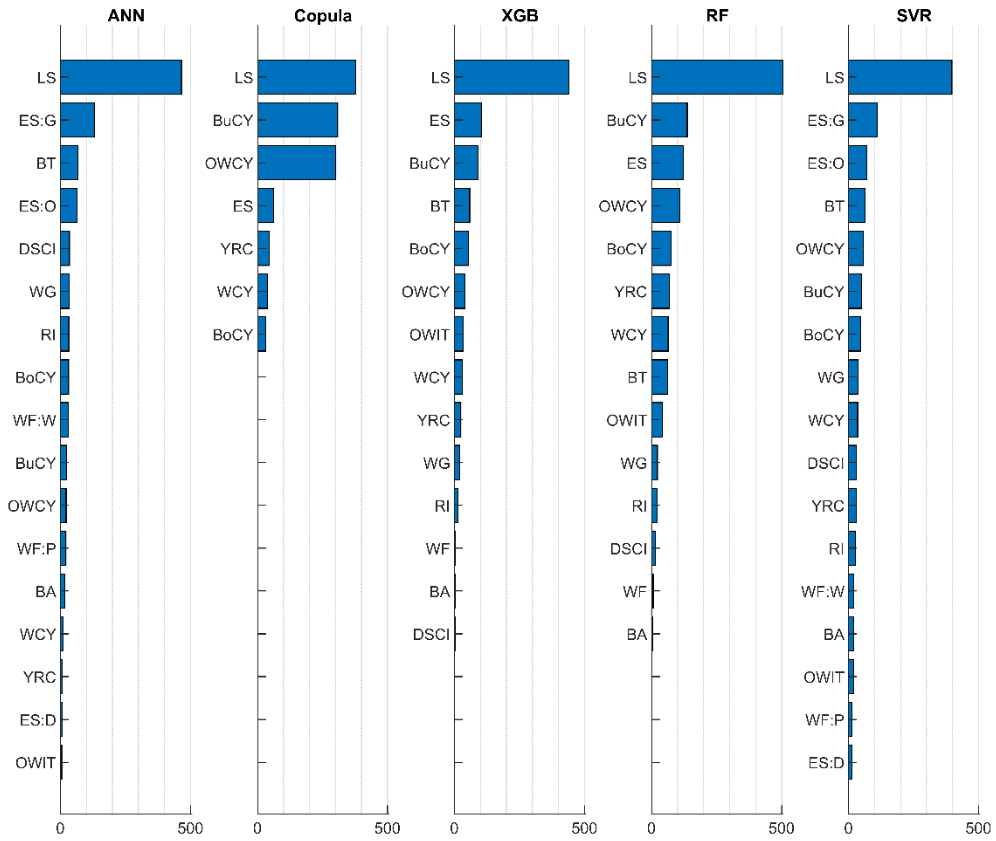

Figure A 2 Complete variable importance plot for the data-driven EQMs (for variable abbreviations see Table A 6)

Table A 6 Variable abbreviations for the variable importance plot in Figure A 2

Attributes	**Key**	**Attributes**	**Key**
Basement available	BA	Boiler construction year	BoCY
Building construction year	BuCY	Building type	BT
Double skin construction insulation	DSCI	Living space	LS
Material of window frame (Wood, plastic, aluminium)	WF: W/P	Outer wall construction year	OWCY
Outer wall insulation thickness	OWIT	Presence of double skin construction insulation	DSCI
Presence of roof insulation	RI	Type of energy source (Oil, gas, district heat, etc.)	ES: G/O/D
Type of window-glazing	WG	Window construction year	WCY
Year of the last roof covering	YRC		