Supervised Machine Learning principles

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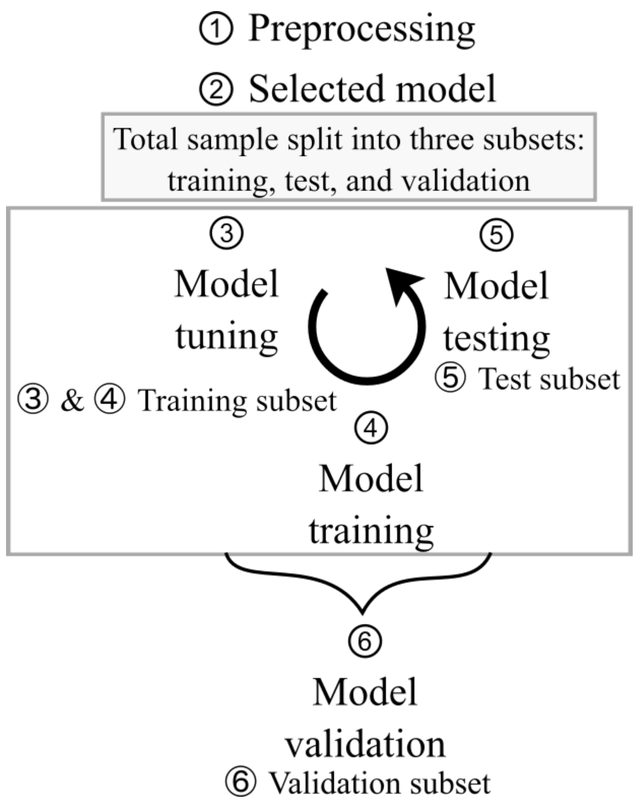
Introduction. Why Supervised Machine Learning (SML)?

S: A target variable **guides** the prediction model's **behavior**.
M: The prediction model runs on a computing **machine**.
L: The prediction model **learns** how the predictors and the target variable are associated, i.e., find optimal trade-off between minimizing prediction errors and maximizing generalizable prediction success.

How does a complete SML process look like?



Demonstration dataset (N = 5)

Predictor values: 4, 9, 10, 12, 15.
Outcome (see SML, target variable) values: 25, 40, 55, 80, 100.

Step 1: Preprocessing

Assuming a nonlinear relationship between predictor and outcome, use the squared predictor values (16, 81, 100, 144, 255).

Step 2: Select model

Select the simple linear regression model.
Split total sample into training, test, and validation subsets:

Obs /Run	1	2	3	4	5
1	V				
2		V			
3			V		
4				V	
5					V

	1.1	1.2	1.3	1.4
2	TE			
3		TE		
4			TE	
5				TE

	2.1	2.2	2.3	2.4
1	TE			
3		TE		
4			TE	
5				TE

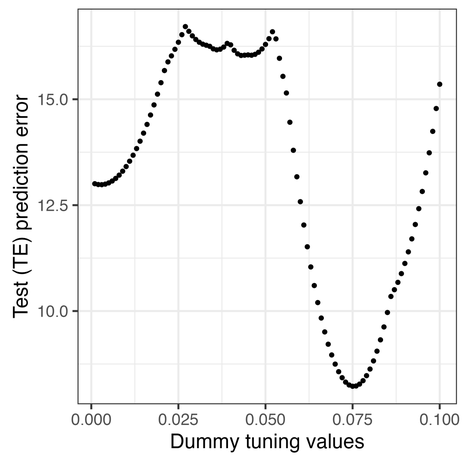
…

	5.1	5.2	5.3	5.4
1	TE			
2		TE		
3			TE	
4				TE

Obs, observation; V, validation; TE, test. Lower tables' empty cells, training.

Step 3: Model tuning

Experimentally influence the training model's regression weight (see SML, find optimal trade-off between bias and variance).



100 different values between 0 and 0.1 were selected for the tuning.

Step 4: Model training. Use training subset (N = 3)

Per training session, add one tuning value to the regression weight.

Step 5: Model testing. Use test subset (N = 1)

Apply each tuned/trained model to the held-out test subset and record the squared prediction error. The lowest prediction error was obtained when adding 0.075 to the regression weight (see step 3).

Step 6: Model validation. Use validation subset (N = 1)

Apply the best test model (TE) to the held-out validation subset (see step 2, upper table) and record the squared prediction error.

Results. Best prediction = lowest squared prediction error.

T–	TE	V	T+	TE	V
Run 1	4.4	41.5	Run 1	0.6	37.0
Run 2	8.9	122.0	Run 2	2.8	205.9
Run 3	41.5	4.4	Run 3	0.5	23.0
Run 4	7.3	132.0	Run 4	23.0	0.5
Run 5	3.1	107.0	Run 5	14.2	74.1
Mn	13.0	**81.4**	Mn	8.2	**68.1**
Md	8.1	**94.2**	Md	5.5	**52.5**

T–, not tuned; TE test; V, validation; T+, tuned; Mn, mean; Md, median.

Tuned better than non-tuned model across the validation subsets.

Conclusion

The six SML principles are meant as a blueprint to eventually master SML introductory texts and scientific reports that apply SML.

Curious? Scan QR code for more SML information ...

Poster content based on: Miché, M., Zander-Schellenberg, T., Wahl, K., & Lieb, R. (2022). *A demonstration of supervised machine learning for psychological researchers* [Manuscript submitted for publication].

A

Obs.	PredictorSq	Outcome
1	16	25
2	81	40
3	100	55
4	144	80
5	225	100

	Run**1**.1	Run**1**.2	Run**1**.3	Run**1**.4
2	81; ?	81; 40	81; 40	81; 40
3	100; 55	100; ?	100; 55	100; 55
4	144; 80	144; 80	144; ?	144; 80
5	225; 100	225; 100	225; 100	225; ?
1	16; ?			

T–	TE	V	T+	TE	V
Run 1	4.4	41.5	Run 1	0.6	37.0
Run 2			Run 2		
Run 3			Run 3		
Run 4			Run 4		
Run 5			Run 5		
Mn	13.0	**81.4**	Mn	8.2	**68.1**
Md	8.1	**94.2**	Md	5.5	**52.5**

B

Obs.	PredictorSq	Outcome
1	16	25
2	81	40
3	100	55
4	144	80
5	225	100

	Run**5**.1	Run**5**.2	Run**5**.3	Run**5**.4
1	16; ?	16; 25	16; 25	16; 25
2	81; 40	81; ?	81; 40	81; 40
3	100; 55	100; 55	100; ?	100; 55
4	144; 80	144; 80	144; 80	144; ?
5	225; ?			

T–	TE	V	T+	TE	V
Run 1			Run 1		
Run 2			Run 2		
Run 3			Run 3		
Run 4			Run 4		
Run 5	3.1	107.0	Run 5	14.2	74.1
Mn	13.0	**81.4**	Mn	8.2	**68.1**
Md	8.1	**94.2**	Md	5.5	**52.5**

Panel **A**: Of four different training models, the second model showed **lowest test** prediction **error** (4.4). Therefore, this (winner) model was cross-validated with the **validation** subset, which yielded the **prediction error** of 41.5. Panel **B**: Same principle, model 3 was winner model.