Deterministic Calibration Function Development

Georgi Tancev

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Case Example: Introduction

- Sensor generates voltage due to reaction(s) with chemical compounds.
- Voltage is proportional to amount of reactants.
- Mapping sensor signal to gas reference concentration ($f : S \to R$), but accounting for cross-sensitivities and other phenomena.

Case Example: Conditions

- The aim is to gather prior information from published data.
- Experimental data from DeVito (2009): Measurement campaign took place at a main street in the center of an Italian city characterized by heavy car traffic.
- Raw sensor data of CO_2, CO, NO_x, NO_2, O_3, temperature, and absolute/relative humidity.
- Reference data of NO_x, NO_2, CO, C_6H_6.
- Each sensor/reference is stationary without replicates and a sampling rate of 1 h^{-1} for a period of one year.
- Is it possible to map raw sensor data to reference, and if yes, how *difficult* is it?

Case Example: Constraints

- Model inference should be feasible with respect to time and space complexity in case model and/or calibration are run locally.
- Backpropagation, which is used for neural network inference, has a time complexity of $\mathcal{O}(n \cdot m \cdot h^k \cdot o \cdot i)$ with n training samples, m features, k hidden layers with h latent variables each, o outputs, and i iterations.
- Gradient descent has time complexity of $\mathcal{O}(n \cdot m \cdot o \cdot i)$, since a neural network without latent variables and with linear activation is equal to a multi-linear regression.
- Stochastic gradient descent has even lower time complexity due to smaller batch size n.
- In addition, space complexity has to be considered as some algorithms are memory-based and need to store all data.
- Ideally, model M_{t-1} from previous calibration time point $t-1$ is retrained by performing several iterations of (stochastic) gradient descent starting from parameters W_{t-1}. This ensures that the new model M_t with parameters W_t does not change too much from its parameter distribution $p(W)$.

Case Example: Workflow

1. Selecting Scikit-Learn (and TensorFlow for comparison) as tool for model development.
2. Starting with a more complex model and trying to predict reference concentrations from sensor voltages.
3. Tuning hyperparameters to obtain a good benchmark.
4. Pruning model by keeping loss approximately constant.
5. Inspecting model to understand its behavior.

Methods: Preprocessing

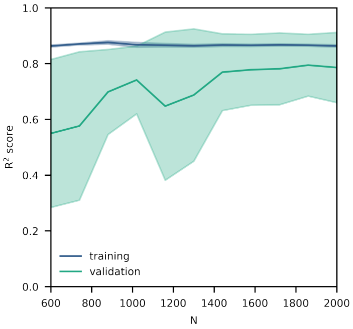
- Drift is unknown, assuming first six months as free from drift and discarding the rest.
- Standard scaling to zero mean and unit variance.
- Dropping missing values instead of imputing.
- Removing outliers with isolation forest.
- Shuffling.
- Final dataset consists of $N = 2'700$ samples over six months.
- Splitting data in $\frac{7}{10}N$ training and $\frac{3}{10}N$ test set.

Methods: Model Development

- Choosing a neural network (multi-layer perceptron) with rectifier activation function as model due to its capability to learn non-linearities.
- Performing a randomized grid search to optimize bias/variance by minimizing mean squared error via 5-fold cross-validation with respect to
  - L_2-regularization parameter $\alpha \in \{10^{-2+0.08j} \mid j \in \mathbb{N}, 0 \leq j \leq 50\}$,
  - number of hidden layers $k \in \{1, 2, 3\}$,
  - and number of latent variables $h \in \{5, 10, 15\}$.
- This leads to a deterministic machine (maximum likelihood estimate), although
  - data is noisy (aleotoric uncertainty)
  - and sensors come from a population (epistemic uncertainty).
- Pruning model by removing layers and latent variables unless loss changes significantly from benchmark.

Results and Discussion

- Final model consists of 1 layer with 10 latent variables and regularization parameter $\alpha = 1.6$
- Amount of data seems reasonable.



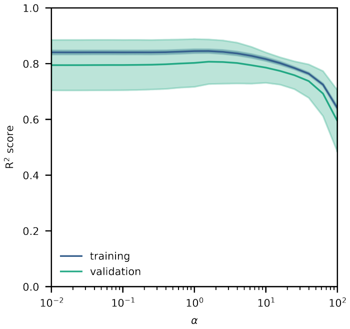
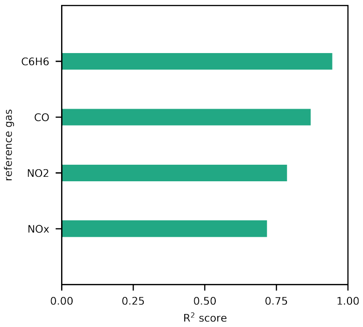


Figure: Training and validation curves for final model.

Results and Discussion

- R^2 score is 0.83, β is 0.81, and mean squared error is 0.10 averaged over all references on test data, which is good compared to literature.
- C_6H_6 has no reference but shows best prediction performance.



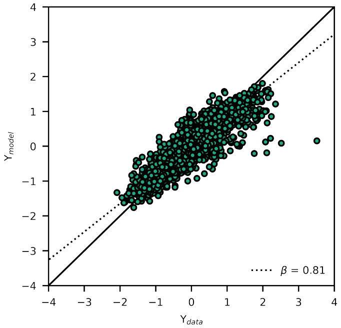
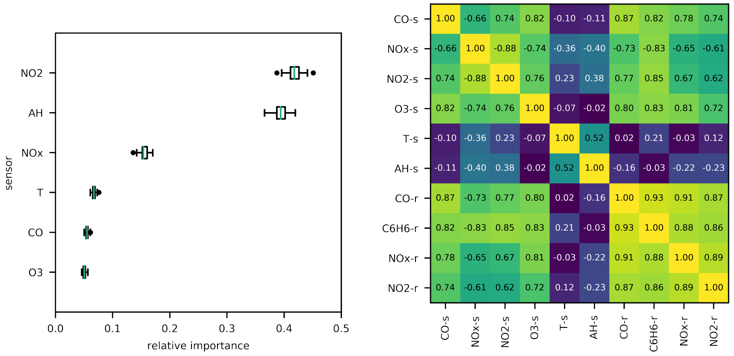


Figure: Model performance with respect to individual references.

Results and Discussion

- Only two sensors are important and rest is apparently redundant.
- The instruments of low importance could suffer from correlations since permutations can be compensated by correlated features.



	CO-s	NOx-s	NO2-s	O3-s	T-s	AH-s	CO-r	C6H6-r	NOx-r	NO2-r
CO-s	1.00	-0.66	0.74	0.82	-0.10	-0.11	0.87	0.82	0.78	0.74
NOx-s	-0.66	1.00	-0.88	-0.74	-0.36	-0.40	-0.73	-0.83	-0.65	-0.61
NO2-s	0.74	-0.88	1.00	0.76	0.23	0.38	0.77	0.85	0.67	0.62
O3-s	0.82	-0.74	0.76	1.00	-0.07	-0.02	0.80	0.83	0.81	0.72
T-s	-0.10	-0.36	0.23	-0.07	1.00	0.52	0.02	0.21	-0.03	0.12
AH-s	-0.11	-0.40	0.38	-0.02	0.52	1.00	-0.16	-0.03	-0.22	-0.23
CO-r	0.87	-0.73	0.77	0.80	0.02	-0.16	1.00	0.93	0.91	0.87
C6H6-r	0.82	-0.83	0.85	0.83	0.21	-0.03	0.93	1.00	0.88	0.86
NOx-r	0.78	-0.65	0.67	0.81	-0.03	-0.22	0.91	0.88	1.00	0.89
NO2-r	0.74	-0.61	0.62	0.72	0.12	-0.23	0.87	0.86	0.89	1.00

Figure: Importance of individual sensors and Spearman rank correlation of signals.

Results and Discussion

- One sensor detects and measures several gases in cases of highly correlated signals and/or references.
- Performing laboratory experiments with varying conditions helps decorrelating signals and removing sampling bias.

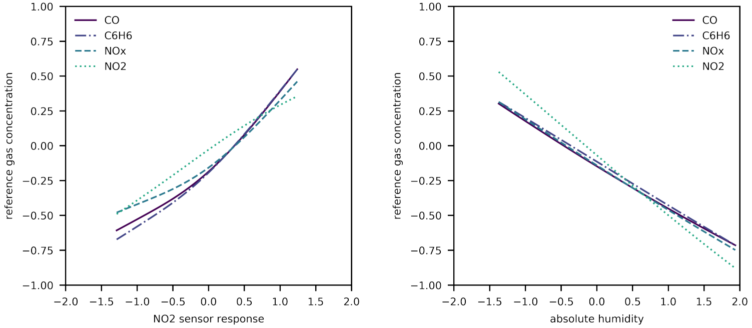


Figure: Partial dependence plots of references on sensors.

Results and Discussion

- Non-linearities are not very pronounced in this particular case.
- Non-linearities can also be modeled using parametric linear models by performing some feature engineering, e.g. basis expansion, or non-parametric random forests with deep trees.

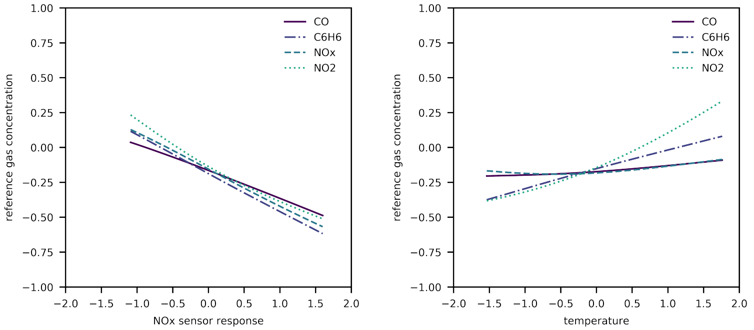


Figure: Partial dependence plots of references on sensors.

Results and Discussion

- Underlying pollutant generation processes are not independent, and hence, chemical concentrations are conditional dependent.

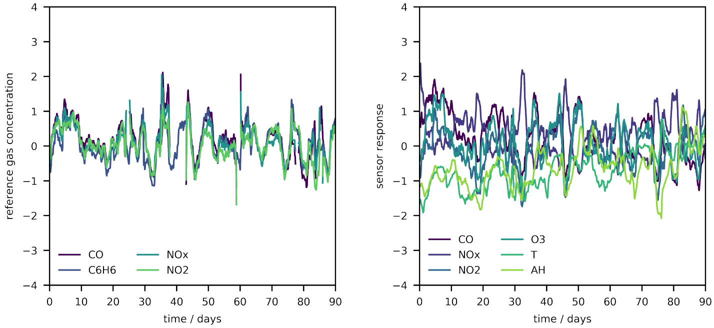


Figure: Time series of references and sensor responses.

Results and Discussion

- Comparison between Scikit-Learn and TensorFlow, since the latter is specialized on graphical models and neural networks.
- Same architecture with early stopping instead of regularization.
- R^2 score is 0.86, β is 0.86, and mean squared error is 0.09 averaged over all references on test data, which is consistent with previous result.

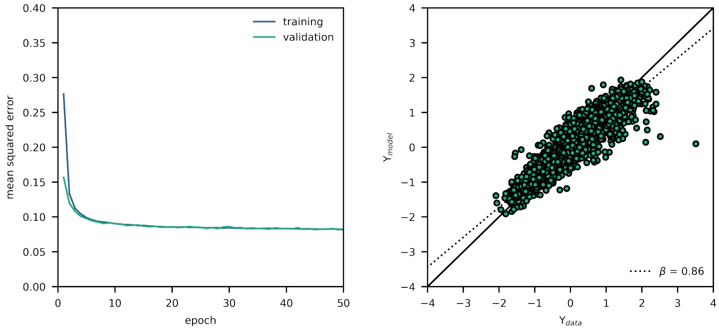


Figure: Model summary with loss and metrics.

Results and Discussion

- Comparison of different algorithms $A = \{$neural network, random forest, linear regression$\}$ is possible.
- Performing basis expansion and hyperparameter optimization to control for bias and variance is mandatory.
- Difference in performance is not that significant compared to time and space complexity.

Table: Model performance on test set data of different algorithms.

metric	**neural network**	**random forest**	**linear regression**
n_i	7	7	27
n_o	4	4	4
hyperparameter(s)	$h,\ k,\ \alpha$	$n_{trees},\ n_{leafs}$	α
mean squared error	0.09	0.09	0.10
R^2	0.86	0.86	0.85
β	0.86	0.82	0.84

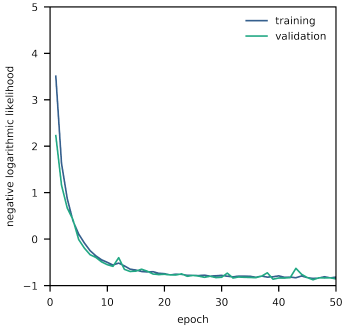
Conclusion

- Inspecting model is a key aspect in machine learning.
- Examining data distribution and quality is of high importance.
- Uniform sampling under laboratory conditions with some design of experiments as complementary data acquisition method is unavoidable for a good model.
- Choice of model class is less likely to be relevant with respect to performance, which would be consistent with the ambiguity in the literature.

Probabilistic Calibration Function Development

Probabilistic Modeling with TensorFlow Probability

- Modeling of aleotoric uncertainty (noise) by Monte-Carlo experiments.
- To obtain a prediction y_i for measurement x_i, k samples from posterior distribution $p(y|x_i)$ are drawn and expectation $y_i = \mu_{y|x_i}$ is calculated.
- Each prediction y_i has information about uncertainty due the standard deviation $\sigma_{y|x_i}$ from the k draws.



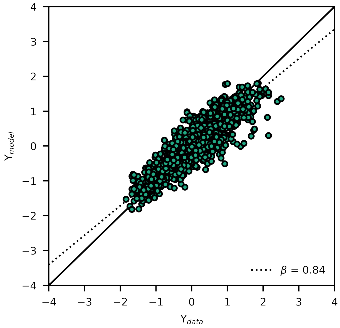


Figure: Model summary with loss and metrics.

Probabilistic Modeling with TensorFlow Probability

- Case example with synthetic time series data from three sensors and three references.
- Prediction is an aggregated result of $\mu_{y|x_i} \pm 1.96 \cdot \sigma_{y|x_i}$ (true value lies in this interval with a probability of 95%).

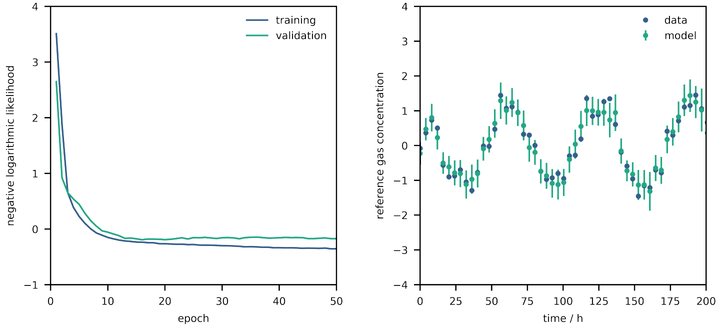


Figure: Training curve with sample prediction.