MACHINE LEARNING REGRESSION ON HYPERSPECTRAL DATA TO ESTIMATE MULTIPLE WATER PARAMETERS

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ABSTRACT
In this paper, we present a regression framework involving several machine learning models to estimate water parameters based on hyperspectral data. Measurements from a multi-sensor field campaign, conducted on the River Elbe, Germany, represent the benchmark dataset. It contains hyperspectral data and the five water parameters chlorophyll a, green algae, diatoms, CDOM and turbidity. We apply a PCA for the high-dimensional data as a possible preprocessing step. Then, we evaluate the performance of the regression framework with and without this preprocessing step. The regression results of the framework clearly reveal the potential of estimating water parameters based on hyperspectral data with machine learning. The proposed framework provides the basis for further investigations, such as adapting the framework to estimate water parameters of different inland waters.

Index Terms— hyperspectral data, machine learning, regression, water parameters, chlorophyll a, CDOM, algae

1. INTRODUCTION

Monitoring the quality of inland waters is a major research topic in many scopes of environmental applications. Traditionally, a water body is monitored with several point-based in-situ measurements. Although, the data measured at such specific points is precise, these measurement techniques are time consuming when covering a large area. Additionally, if area-wide information is required, the data needs to be interpolated as well. Regarding the demand for area-wide information of water parameters, hyperspectral sensing seems to close the gap left behind by in-situ point-measurements.

The spectral signature of natural water bodies is mainly characterized by absorption and scattering on four water parameters: chlorophyll a, suspended solids, colored dissolved organic matter (CDOM) and turbidity [1, 2]. Chlorophyll a is a pigment which functions as an indicator for algae existence and nutrition supply in water bodies. Turbidity is influenced by algae concentrations and suspended particles. CDOM is a natural degradation product group of organic materials which is natural in waters. It is also affected by human impacts like sewage treatment plants.

Recent approaches were made to estimate chlorophyll a concentration, CDOM content and turbidity with hyperspectral data. As described in [1], the spectral signature of chlorophyll a in water is characterized by a reflectance minimum at about 670 nm as well as reflectance maxima in the green and red spectral range. The distinction of algae species based on their measured hyperspectral signature was studied e.g. in a laboratory [2]. With increasing CDOM content, the absorption simultaneously increases in shorter wavelengths [3].

Estimations of water parameters with hyperspectral data mostly rely on empirical approaches. Centerpiece of these approaches is, on the one hand, the selection of reflectance bands including single bands, band ratios and multiple band algorithms [3, 4, 5, 6, 7, 8, 9, 10, 11]. On the other hand, further studies consider the area between 672 nm to 742 nm under the related maximum [12, 13] or the maximum itself [1, 12, 13] for the estimation of chlorophyll a concentration. In addition, derivatives of the spectra up to the fourth grade are applied [5, 11].

Machine learning approaches to estimate CDOM and chlorophyll a are applied yet solely in few studies. The former is estimated with e.g. functional linear models [14] or linear stepwise regression [15]. Currently, random forests are applied to estimate the latter [16]. In general, machine learning models require sufficient input data to solve a non-linear regression problem with high-dimensional data.

In this paper, we proceed to examine the potential of supervised machine learning approaches to estimate crucial water parameters such as chlorophyll a, green algae, diatoms, CDOM, and turbidity. We rely on a dataset which was measured on the German part of the River Elbe under real-world conditions. Precise monitoring of the water parameters followed by hyperspectral snapshots and in-situ probe measurements were conducted. As a remark, a first impression and a
description of the dataset is given in [16].

The major contributions of this paper are:

• a detailed analysis of the potential of hyperspectral data to estimate these water parameters;
• an adequate framework with five regression models: k-nearest neighbor (k-NN), random forest (RF), support vector machine (SVM), multivariate adaptive regression splines (MARS) and extreme gradient boosting (XGB);
• an comprehensive evaluation of the regression performance with and without preprocessing.

We briefly describe the dataset used for the estimation of water parameters based on the introduced regression framework in Section 2. The presentation of the methodology follows in Section 3. We assess the regression performance of the five machine learning models in Section 4. Finally, we briefly conclude our studies in Section 5.

2. DATASET

To evaluate the potential of hyperspectral data as input data for the estimation of water parameters, we rely on a dataset which was sampled during a field campaign in summer 2017 on the River Elbe. A hyperspectral sensor Cubert UHD 285 was mounted on a research ship. The PhycoSens sensor, an invention of BBE Moldaenke, sampled the concentration of chlorophyll $a$, green algae and diatoms. Additionally, the Biofish sensor system [17] measured the concentration of CDOM and the turbidity. The distributions of the measured water parameters are illustrated in Fig. 1. A detailed description of the actual data acquisition is presented in [16].

As for the hyperspectral snapshot data, each image contains $50 \times 50$ pixels and 125 spectral channels ranging from 450 nm to 950 nm with a spectral resolution of 4 nm. A selection of the hyperspectral bands is applied to avoid sensor artifacts. This results in a range of wavelengths from 470 nm to 910 nm. Furthermore, the measured mean spectra of all images were calculated by manually selecting an area, which was undisturbed by bubble formations, shadows or waves.

The sampled reference data of the PhycoSens data is extended by a linear interpolation. This interpolation is appropriate, since the measured concentrations change in a continuous matter. The dataset emerging of the measurements with the PhycoSens counts 1163 high-dimensional datapoints defined by selected hyperspectral bands and the concentrations of chlorophyll $a$, green algae as well as diatoms as reference data. Hyperspectral datapoints, which are convenient to the Biofish sensor system data, consist of 802 values combining selected hyperspectral bands, CDOM, and turbidity as references.

3. METHODOLOGY

To estimate water parameters with hyperspectral data, we use the given dataset for our proposed regression framework. We apply five supervised machine learning models: k-nearest neighbor (k-NN), random forest (RF), support vector machine (SVM), multivariate adaptive regression splines (MARS) and extreme gradient boosting (XGB). They perform the regression with the hyperspectral data as input vector and the respective water parameter as target value. Table 1 provides a brief summary of all model implementations.

The datasets (cf. Section 2) are split into a training and a test subset in a ratio of $3 : 7$. All models of the framework are trained on the respective training subset and are evaluated on the respective test subset. For a reasonable estimation of each water parameter, the distributions of the subsets have to be representative of the specific water parameter’s distribution. The split ratio as well as the distinction between training and test subset decrease overfitting. Fig. 1 provides histograms of the distribution of each water parameter.

To reduce the dimensionality of the hyperspectral input data, we apply a principal component analysis (PCA) as a preprocessing step. We choose the first eight principal components to fit the models since they cover 99.9% of the overall variability. Alternatively, the regression framework performs the estimation of the water parameters without PCA to which we refer as raw bands in Section 4. With respect to the k-NN, SVM, and MARS regression models, the input data always is scaled [18, 19, 20].
4. RESULTS

The regression results of the framework for the estimation of the five water parameters are summarized in Fig. 2. The regression performance is expressed in terms of the coefficient of determination ($R^2$) and the root mean squared error (RMSE). The results reveal that the five regression models estimate all water parameters with solely hyperspectral input data remarkably well. Tables 2 to 6 contain the regression results sorted by water parameters. In total, RF, SVM and k-NN models perform better than the MARS and XGB models.

The best estimation performance of each model is obtained by applying the PCA as preprocessing step. The chlorophyll $a$ and CDOM concentrations are estimated well by the regression framework (cf. Tables 2 and 4). Each model reaches $R^2$ of approximately 90% with PCA. The estimation performances of diatoms, green algae, and turbidity concentrations achieve $R^2 > 80\%$ with PCA (cf. Tables 3, 4 and 6).

The MARS regression model performs worst compared to the others. RF provides the best performances of estimating CDOM while the best estimation of the turbidity is achieved by the SVM regression. The SVM and the k-NN model outperform the other models when estimating the concentrations of chlorophyll $a$, green algae, and diatoms. We point out, that outliers in the distribution of the reference data (cf. Fig. 1) might influence any regression results.

5. CONCLUSION

In this paper, we address the estimation of water parameters with hyperspectral data. In contrast to most approaches modeling such water parameters, we apply machine learning models. Our major objective is to evaluate the potential of such models when estimating the amount of chlorophyll $a$, green algae, diatoms, CDOM or turbidity in inland waters.

We introduce a regression framework involving five selected machine learning models. As benchmark data, we rely on a dataset, conducted on the River Elbe in Germany which is characterized by measurements of five distinct water parameters. The regression is conducted with and without PCA to evaluate the impact of dimensionality reduction on the performance due to the applied dimensionality reduction of the input data. The regression results of the framework clearly reveal the potential of estimating water parameters based on hyperspectral data with machine learning.

The advantages of this framework, in contrast to commonly applied methods, e.g. band ratios, is the ability of machine learning to handle high-dimensional regression problems. This ability is even given when performing on small, measured datasets. To conclude our regression framework serves as starting point for further investigations like adapting the framework to estimate water parameters of different types of inland waters.

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### Table 1: Implementations of the regression models with the respective R packages.

| Regression model | Package | Reference |
|------------------|---------|-----------|
| k-NN             | caret   | [18]      |
| RF               | ranger  | [21, 22]  |
| SVM              | e1071   | [19]      |
| MARS             | earth   | [20]      |
| XGB              | xgboost | [23]      |

### Table 2: Regression results of the framework for chlorophyll $a$ estimation.

| Model  | raw bands | with PCA |
|--------|-----------|----------|
|        | $R^2$     | RMSE     | $R^2$     | RMSE     |
|        | in %      | in $\mu$g/L | in %      | in $\mu$g/L |
| k-NN   | 74.7      | 17.2     | 92.8      | 9.1      |
| RF     | 78.1      | 16.1     | 90.7      | 11.5     |
| SVM    | 89.7      | 10.9     | 93.9      | 8.3      |
| MARS   | 89.5      | 11.2     | 88.8      | 11.4     |
| XGB    | 79.7      | 15.3     | 91.8      | 9.7      |

### Table 3: Regression result of the framework for green algae estimation.

| Model  | raw bands | with PCA |
|--------|-----------|----------|
|        | $R^2$     | RMSE     | $R^2$     | RMSE     |
|        | in %      | in $\mu$g/L | in %      | in $\mu$g/L |
| k-NN   | 61.1      | 13.2     | 88.9      | 7.1      |
| RF     | 67.5      | 12.2     | 82.1      | 9.4      |
| SVM    | 77.6      | 10.0     | 88.6      | 7.2      |
| MARS   | 76.7      | 10.2     | 76.8      | 10.2     |
| XGB    | 67.9      | 12.0     | 82.6      | 8.8      |

### Table 4: Regression result of the framework for diatoms estimation.

| Model  | raw bands | with PCA |
|--------|-----------|----------|
|        | $R^2$     | RMSE     | $R^2$     | RMSE     |
|        | in %      | in $\mu$g/L | in %      | in $\mu$g/L |
| k-NN   | 64.6      | 11.5     | 89.8      | 6.2      |
| RF     | 69.7      | 10.9     | 86.1      | 8.1      |
| SVM    | 78.3      | 9.0      | 88.8      | 6.5      |
| MARS   | 79.2      | 8.9      | 81.8      | 8.2      |
| XGB    | 68.6      | 10.8     | 87.3      | 7.0      |
Fig. 2: Regression results for the estimation of the water parameters expressed as $R^2$ without PCA (left) and with PCA (right).

Table 5: Regression result of the framework for CDOM estimation. CDOM is measured in parts per billion, $\text{ppb}_{\text{QS}} = 10^{-9}$ and is calibrated against Quinine Sulfate (QS).

| Model | raw bands | with PCA |
|-------|-----------|----------|
|       | $R^2$ in % | RMSE in $\text{ppb}_{\text{QS}}$ | $R^2$ in % | RMSE in $\text{ppb}_{\text{QS}}$ |
| k-NN  | 82.4      | 0.9      | 91.9      | 0.6 |
| RF    | 84.3      | 0.8      | 94.1      | 0.5 |
| SVM   | 91.1      | 0.6      | 93.3      | 0.5 |
| MARS  | 90.7      | 0.6      | 89.9      | 0.7 |
| XGB   | 82.2      | 0.9      | 91.4      | 0.6 |

Table 6: Regression result of the framework for turbidity estimation. The turbidity is measured in Formazin Turbidity Unit (FTU).

| Model | raw bands | with PCA |
|-------|-----------|----------|
|       | $R^2$ in % | RMSE in FTU | $R^2$ in % | RMSE in FTU |
| k-NN  | 70.0      | 0.3      | 88.8      | 0.2 |
| RF    | 72.3      | 0.2      | 88.6      | 0.2 |
| SVM   | 83.0      | 0.3      | 90.2      | 0.2 |
| MARS  | 75.1      | 0.3      | 83.7      | 0.2 |
| XGB   | 65.9      | 0.3      | 83.2      | 0.2 |

6. REFERENCES

[1] Anatoly A. Gitelson and G. P. Keydan, “Remote Sensing of Inland Surface Water Quality - Measurements in the Visible Spectrum,” *Acta hydrophys.*, vol. 34, pp. 5–27, 1990.

[2] Peter D. Hunter, Andrew N. Tyler, Matyas Presing, Attila W. Kovacs, and Tom Preston, “Spectral discrimination of phytoplankton colour groups: The effect of suspended particulate matter and sensor spectral resolution,” *Remote Sensing of Environment*, vol. 112, no. 4, pp. 1527–1544, 2008.

[3] Kevin D. Menken, Patrick L. Brezonik, and Marvin E. Bauer, “Influence of Chlorophyll and Colored Dissolved Organic Matter (CDOM) on Lake Reflectance Spectra: Implications for Measuring Lake Properties by Remote Sensing,” *Lake and Reservoir Management*, vol. 22, no. 3, pp. 179–190, 2006.

[4] Anatoly A. Gitelson, “The peak near 700 nm on radiance spectra of algae and water: Relationships of its magnitude and position with chlorophyll concentration,” *International Journal of Remote Sensing*, vol. 13, no. 17, pp. 3367–3373, 1992.

[5] Donald C. Rundquist, Luoheng Han, John F. Schalles, and Jeffrey S. Peake, “Remote Measurement of Algal Chlorophyll in Surface Waters: The Case for the First Derivative of Reflectance Near 690 nm,” *Photogrammetric Engineering & Remote Sensing*, vol. 62, no. 2, pp. 195–200, 1996.
[6] R. N. Fraser, “Hyperspectral remote sensing of turbidity and chlorophyll a among Nebraska Sand Hills lakes,” International Journal of Remote Sensing, vol. 19, no. 8, pp. 1579–1589, 1998.

[7] Sampsa Koponen, Jouni Pulliainen, Kari Kallio, and Martti Hallikainen, “Lake water quality classification with airborne hyperspectral spectrometer and simulated MERIS data,” Remote Sensing of Environment, vol. 79, no. 1, pp. 51–59, 2002.

[8] Asif M. Bhatti, Donald C. Rundquist, John F. Schalles, Luis Ramirez, and Seigo Nasu, “Application of hyperspectral remotely sensed data for water quality monitoring: accuracy and limitation,” Accuracy 2010 - Proceedings of the 9th International Symposium on Spatial Accuracy Assessment in Natural Resources and Environmental Sciences, pp. 349–352, 2010.

[9] Mark W. Matthews, Stewart Bernard, and Kevin Winter, “Remote sensing of cyanobacteria-dominant algal blooms and water quality parameters in Zeekoevlei, a small hypertrophic lake, using MERIS,” Remote Sensing of Environment, vol. 114, no. 9, pp. 2070–2087, 2010.

[10] Liguo Zhou, Bo Xu, Weichun Ma, Bin Zhao, Linna Li, and Hongyan Huai, “Evaluation of Hyperspectral Multi-Band Indices to Estimate Chlorophyll-A Concentration Using Field Spectral Measurements and Satellite Data in Dianshan Lake, China,” Water, vol. 5, no. 2, pp. 525–539, 2013.

[11] Mak Kisevic, Mira Morovic, and Roko Andircevic, “The use of hyperspectral data for evaluation of water quality parameters in the River Sava,” Fresenius environmental bulletin, vol. 25, no. 11, pp. 4814–4822, 2016.

[12] Sandra Mannheim, Karl Segl, Birgit Heim, and Hermann Kaufmann, “Monitoring of lake water quality using hyperspectral CHRIS-PROBA data,” Proceeding of the 2nd CHRIS/Proba Workshop, ESA/ESRIN, 2004.

[13] John F. Schalles, Anatoly A. Gitelson, Yosef Z. Yacobi, and Amy E. Kroenke, “Estimation of chlorophyll a from time series measurements of high spectral resolution reflectance in an eutrophic lake,” Journal of Phycology, vol. 34, no. 2, pp. 383–390, 1998.

[14] Qian Yu, Yong Q. Tian, Robert F. Chen, Anna Liu, G. Bernard Gardner, and Weining Zhu, “Functional Linear Analysis of in situ Hyperspectral Data for Assessing CDOM in Rivers,” Photogrammetric Engineering & Remote Sensing, vol. 76, no. 10, pp. 1147–1158, 2010.

[15] Patrick L. Brezonik, Leif G. Olmanson, Jacques C. Finlay, and Marvin E. Bauer, “Factors affecting the measurement of CDOM by remote sensing of optically complex inland waters,” Remote Sensing of Environment, vol. 157, pp. 199–215, 2015.

[16] Philipp M. Maier, Stefan Hinz, and Sina Keller, “Estimation of Chlorophyll a, Diatoms and Green Algae Based on Hyperspectral Data with Machine Learning Approaches,” 38. Wissenschaftlich-Technische Jahrestagung der DGPF und PFGK18 Tagung in München, vol. 27, pp. 49–57, 2018.

[17] Andreas Holbach, Stefan Norra, Lijing Wang, Yuan Yijun, Wei Hu, Binghui Zheng, and Yongsong Bi, “Three Gorges Reservoir: Density pump amplification of pollutant transport into tributaries,” Environmental science & technology, vol. 48, no. 14, pp. 7798–7806, 2014.

[18] N S Altman, “An introduction to kernel and nearest-neighbor nonparametric regression,” The American Statistician, vol. 46, no. 3, pp. 175, 1992.

[19] Vladimir N. Vapnik, The Nature of Statistical Learning Theory, 1995.

[20] Jerome H. Friedman, “Multivariate adaptive regression splines,” The Annals of Statistics, vol. 19, no. 1, pp. 1–67, 1991.

[21] Leo Breiman, “Random forests,” Machine Learning, vol. 45, no. 1, pp. 5–32, 2001.

[22] Pierre Geurts, Damien Ernst, and Louis Wehenkel, “Extremely randomized trees,” Machine Learning, vol. 63, no. 1, pp. 3–42, 2006.

[23] Jerome H. Friedman, “Greedy function approximation: A gradient boosting machine,” The Annals of Statistics, vol. 29, no. 5, pp. 1189–1232, 2001.