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From Hyperspectral to Multispectral Sensing and from Simulation to Reality: A Comprehensive Approach to Calibration Model Transfer

Patrick Menz[1*], Valerie Vaquet[2*], Barbara Hammer[2], and Udo Seiffert[1§]

1- Cognitive Processes and Systems, Fraunhofer Institute for Factory Operation and Automation IFF, Magdeburg – Germany
2- Machine Learning Group Bielefeld University, Bielefeld - Germany

Abstract. High-resolution hyperspectral sensors provide precise but expensive information on an object's chemical composition in various industries. We present a method for transferring this capability to customized low-cost multispectral solutions. Taking a relevance analysis of spectra for a given problem as our starting point, we simulated and designed a multispectral sensor based on inverse spectroscopy. The corresponding calibration model, which was derived from the simulation of such a multispectral sensor and connected with its hardware, may not drop in precision significantly. Different methods of calibration model transfer capable of handling a limited subset of the data were tested for this purpose. The latent space transformation with Chebyshev polynomials outperformed all other methods by yielding the fewest labeled data.

1 Introduction

Hyperspectral sensing is a noninvasive alternative to wet chemistry for identifying biochemical processes and properties of objects. It is increasingly being used in different fields, such as quality control, agriculture, forensics and remote sensing [1]. The cost and sensitivity of hyperspectral sensors make them impracticable for many applications, including sensor-controlled consumer IoT devices. Many applications do not require the complete spectral signature from a high-precision hyperspectral sensor to constitute a suitable technical solution. A multispectral sensor system using a subset of spectral bands customized for the underlying application can often close this gap [2].

A mathematical calibration model is used to convert spectral signatures into information relevant to the application. Depending on the type of application, this may be a classifier or a regression model. The calibration model correlates the spectral data with application-specific target data. Since this correlation normally cannot be displayed analytically, methods of machine learning are used for this purpose.

Information on the actual wavelengths required is essential to the transition from hyperspectral to multispectral sensor technology. Usually, extensive sets of samples are recorded with a high-precision hyperspectral reference sensor and an initial calibration model is calculated for this purpose. This furnishes two essential pieces of information. First, an upper estimate of how well the existing measurement task can be implemented at all with the most precise data potentially available, and, second, whenever relevance

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[§] Present address: Compolytics GmbH, Barleben - Germany

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learning methods are used, an application-specific relevance profile. This identifies the input variables of the high-dimensional hyperspectral data space, which are actually needed or used by the specific calibration model. Subsequent interpretation of this relevance profile delivers the spectral design needed for the application-specific multispectral sensor.

This custom sensor can be simulated by transforming the high-dimensional signature of the hyperspectral sensor [3]. The simulation can be used to estimate the loss of recognition performance related to the transition from the hyperspectral to the multispectral sensor. Once this has been done, construction of the real multispectral sensor can begin. Manufacturers' data sheets often provide the spectral signatures of the available optical components, especially filters and, when inverse spectroscopy is used (see Section 2.2), of corresponding LEDs. These can be used in the simulation in this paper (see Section 2.3). The general dilemma is that the physical samples from the initial measurement trial are no longer available or that extensive new measurements with the hardware sensor built would be too expensive. Only the repeated measurement of a few labeled samples for the transfer and its validation is acceptable.

Ultimately, there are three levels of sensors, (1) the hyperspectral sensor with a complete high-resolution signature, (2) the simulated multispectral sensor supplying the theoretically calculated reduced signature of (1) based on data sheets of available optical components and (3) the multispectral sensor that can be built into hardware. This paper uses a specially designed benchmark application to analyze the precision of these three sensor levels, focusing on different approaches to transferring the calibration model from simulation (2) to reality (3) by using only a subset of labeled samples, as presented in Figure 1. Standard mathematical methods [4], and the authors' experience with model transfer in the context of interoperability [5, 6] are used to do this.

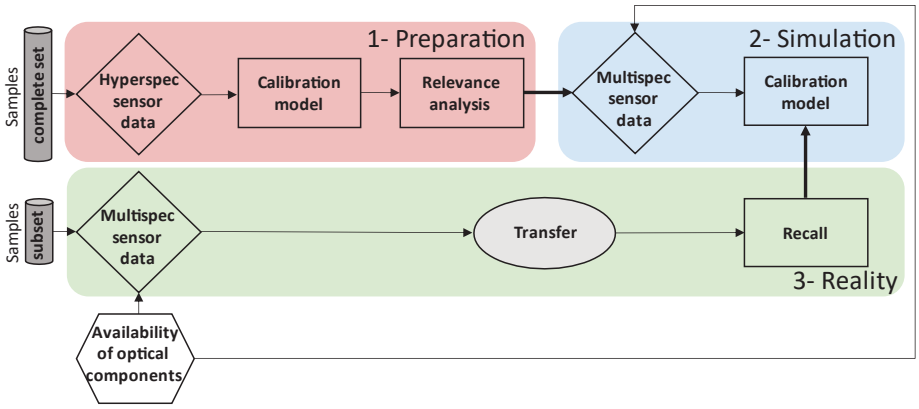

Fig. 1: Diagram of the proposed procedure, colored boxes signifying the main steps. 1-Preparation using the complete set of samples measured by a hyperspectral sensor to identify features relevant to the application. 2-Simulation of a multispectral sensor incorporating commercially available optical components and calibration model training. 3-Reality, i.e., the building of the multispectral sensor and the measuring of a subset of the samples used for transfer to transfer the calibration model from simulation to reality.

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2 From Hyperspectral to Multispectral

Although hyperspectral measurement technology frequently constitutes the optimal solution in many fields of application, it entails high capital expenditures. Hyperspectral sensors are usually expensive and therefore impracticable for consumer applications. We use an application-specific multispectral measurement technology, though, the development of which we present in this section.

Data set. We painted ten metal plates with RAL 3000 fire red paint sourced from ten different manufacturers, thus creating a functional 10-class problem in which we want to identify the different manufactures. Despite having the same color code, the paints themselves have different compositions of different pigments, solvents and binders. This benchmark data and the corresponding classification task could be used in various application scenarios, such as product authenticity testing, repainted car part detection, and general quality control.

An ASD FieldSpec® 4 Wide-Res (hereafter called FieldSpec) was used as a high-precision hyperspectral measuring device, which measures 2,151 spectral bands in the range of 350nm and 2,500nm. We measured different locations on each of the ten metal plates ten times since the painting can vary within a class. This yielded 100 samples.

Sensor engineering. We employed the technique of inverse spectroscopy to design a low-cost sensor to replace an expensive hyperspectral sensor. Whereas conventional spectral measurement systems normally use broadband illumination (halogen) and a narrowband sensor, inverse spectroscopy uses narrowband illumination (LED) and a broadband receiver, instead. The advantage of inverse spectroscopy is that its electronic components, such as LEDs, photodetectors and ADCs, are easily incorporated in mobile devices and thus affordable for consumer applications. Although inverse spectroscopy results in a lower resolution than our FieldSpec, for instance, such a large number of spectral bands and this bandwidth are rarely needed to solve a classification or regression problem.

The first (red) box in Figure 1 shows the procedure we used in this paper. A relevance analysis of the complete spectral signature based on feature importance in an RBF network identified the number of wavelengths needed for the calibration model to solve the classification problem [2]. Ten wavelengths proved to be all that are needed.

A multispectral sensor suitable for this task was easily constructed using a LED and detector combination with the principle of inverse spectroscopy, which measures the ten requisite wavelengths, and LED emission and photodetector sensitivity curves provided by the manufacturer.

Multispectral simulation. Before the real sensor was built, it was simulated (hereafter called simulated sensor) to predict the calibration model's performance with the multispectral data generated. The simulated spectrum R_{sim} is composed as follows:

$$R_{sim} = \int E_{led} \cdot S_{detec} \cdot R_{full} \, d\lambda \,, \tag{1}$$

where E_{led} describes the emission curve of each individual LED, S_{detec} the sensitivity curve of each individual detector and R_{full} the spectrum of the FieldSpec.

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We measured the data set with the real device built to evaluate transfer performance in this study. As with the FieldSpec, we again recorded 100 measuring points, which have just ten spectral bands in the range of 400-1,000 nm, though. The data set is thus complete for each of the three sensors, i.e., the FieldSpec (1), the simulated sensor (2) and the real sensor (3), which, as was mentioned in the introduction, are needed to transfer the calibration model from (2) to (3).
We detect slight differences when comparing the simulated spectra with the real spectra, which will affect our classifier's performance (see Figure 2).

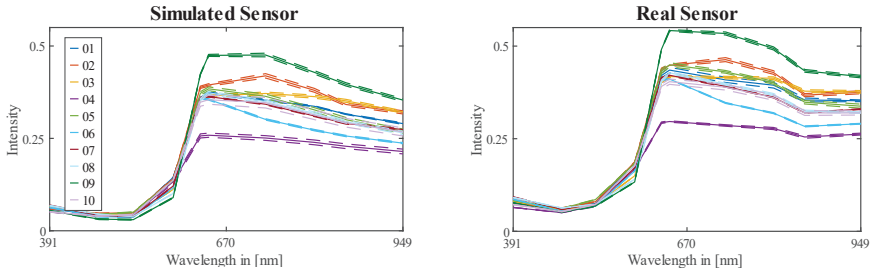

Fig. 2: Mean spectral signal of each sample, displaying reasonably low STD (dotted line).

There are several reasons for this. For instance, each LED is a unique optical component subject to changes not specified in data sheets. Furthermore, LEDs and other electronic sensor components are sensitive to temperature change. This causes intensity and transversal drift in our spectra, something treated in [6]. Robust methods against drifts are presented in [6] and briefly covered in Section 3.

3 Calibration Model Transfer

The motivation for calibration model transfer is the need for a calibration model based on machine learning, which has been learned by a "master" spectral sensor (in this study, the simulated sensor (2)), to perform well even when data is transmitted from a different "slave" sensor (in this study, the real sensor (3)). The calibration transfer methods employed in this study are presented briefly below.

Piecewise direct standardization. Often used in chemometrics, piecewise direct standardization (PDS) is a method for transferring a calibration model from one spectral sensor to another [4, 8]. A transformation matrix is calculated by crosschecking one sensor's spectra with another sensor's spectra for a few adjacent wavelengths. This method is able to handle intensity and transversal drifts.

Offset elimination. As the name indicates, this method eliminates offsets that intensity and transversal shift can cause. A simplification of the transfer component analysis [8] is adopted in this paper, which is intended to optimize the maximum mean discrepancy. This simplification necessitates standardizing each data set component-wise. We ultimately subtract the mean spectrum for each sensor in every sample[6].

Latent space transformation with Chebyshev polynomials. The effectiveness of Chebyshev polynomials in the transformation of spectra has been demonstrated in [9].

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The model trained with coefficients of Chebyshev polynomials, representing a latent space, rather than with spectra. This method's suitability for dealing with shifts has been demonstrated in [6]. In our study, the data in the latent space were z-transformed to normalize the large differences of the Chebyshev coefficients. We call this the Chebyshev method.

Transfer learning with tRBF. A transfer learning method specially developed for an RBF network was used in [5] to demonstrate the transferability of spectral sensor data in different camera systems. There was one drawback, though: Classes could not be omitted during transfer learning in [5]. Data from all the classes involved were repeatedly needed, even though training was possible with significantly fewer samples.

4 Results

An RBF network with ten prototypes was used as the classification model. This base model was subjected to a 10-fold cross-validation. The average classification rates are presented below. All models achieved a classification performance of 100% without an involved sensor transfer (FieldSpec (1), simulated sensor (2) and real sensor (3)). We analyze the results of the model trained with (2) for the data from (3) (see Figure 1). We used three samples per class for our transfer. Ten coefficients were computed for the Chebyshev method to approximate each spectrum.

Different numbers of classes and thus labeled samples were used to analyze the effect of incomplete data on the transfer (Figure 1). A maximum of 30 labeled samples for all ten classes and three samples per class were used for our transfer, leaving 70 for validation. We repeated our experiment ten times to verify the robustness of the transfer as a function of classes used, selecting the classes randomly with a fixed seed to ensure the same classes were used for each transfer method. The use of one class for each transfer ultimately means that each class of our dataset was used once.

Figure 3 presents the results of the transfer methods analyzed as a function of the number of classes used.

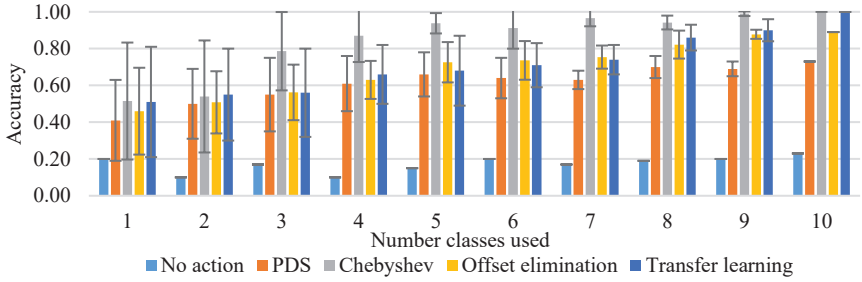

Fig. 3: Results of the transfer using real sensor data processed in a simulated sensor calibration model as a function of the classes used. The colored bars represent the mean values of ten experiments and the error bars denote the standard deviation.

A larger number of classes is associated with higher costs. The labels for plant samples, for instance, come from expensive wet chemical analyses.

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Transfer learning and the Chebyshev method both deliver the original classification accuracy of 100% when all classes are used for the transfer. Offset elimination delivers good results too. All the same, the Chebyshev method already delivers satisfactory results when just five classes are used, thus making it the best method for this application. We can also see, however, that the standard deviation for the classes used, numbering as many as seven, is high. This indicates that the selected classes affect the transfer process significantly.

5 Conclusion

In this study, we have demonstrated the replacement of an expensive hyperspectral sensor with an application-specific and affordable multispectral sensor. We have also presented the simulation of such a multispectral sensor's spectral response and use the data for a corresponding calibration model based on machine learning. Moreover, a calibration model was transferred from the simulated multispectral sensor to a real sensor and evaluated as a function of the classes used for the transfer. Latent space transformation with Chebyshev polynomials combined with z-transformation proved to deliver the best results for our application. Future research ought to incorporate interoperability, whenever there is more than one real sensor, and a data set with larger intraclass variance.

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