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Utilizing support vector and kernel ridge regression methods in spectral reconstruction

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ABSTRACT

Two regression methods, namely, Support Vector Regression (SVR) and Kernel Ridge Regression (KRR), are used to reconstruct the spectral reflectance curves of samples of Munsell dataset from the corresponding CIE XYZ tristimulus values. To this end, half of the samples (i.e., the odd ones) were used as training set while the even samples left out for the evaluation of reconstruction performances. Results were reviewed and compared with those obtained from Principal Component Analysis (PCA) method, as the most common context-based approach. The root mean squared error (RMSE), goodness fit coefficient (GFC), and CIE LAB color difference values between the actual and reconstruct spectra were reported as evaluation metrics. However, while both SVR and KRR methodologies provided better spectral and colorimetric performances than the classical PCA method, the computation costs were considerably longer than PCA method.

1. Introduction

The spectral reflectance of any object is known as a non-repetitive component that provides full information about the color of the object under different viewing conditions. Hence, having access to this information is crucial in various industries that deal with colors and colorants. This information can be used in many fields, such as device color characterization, color matching efforts and the most important one, i.e., material identification. Compared to color measurement devices like RGB cameras, the reflection measuring devices such as spectrophotometers and spectral cameras are not widely available and are more professional and relatively expensive. This limits the use of spectral devices to research and/or industrial laboratories (Abed et al., 2009). So, an acceptable approximation of spectral data from the more accessible colorimetric coordinates such as RGB or standard CIE XYZ information has been an attractive research subject in color science field, and various context and non-context-based approaches such as principal component analyzing (PCA), non-negative matrix factorization (NMF) and pre-defined Gaussian additive primaries have been introduced for this purpose (Wu et al., 2015; Agahian et al., 2008; Amirshahi and Amirhahi, 2010; Harifi et al., 2008; Hawkyard, 1993; Eslahi et al., 2009). The importance of reflectance models in computer graphics is also crucial for multispectral imaging systems where different image-based reflectance estimation techniques have been developed. In this type of application, the spectral data can be reconstructed from the response of the corresponding multi-channel imaging system (Xu and Xu, 2016). In this regard, many research studies have been directed in the recent decades toward reconstruction of spectral reflectances of objects based on camera responses using different supervised and unsupervised methods (Xu and Xu, 2016; Zhou et al., 2020; Heikkinen et al., 2008; Wei et al., 2022; Shimano, 2006; Peyvandi et al., 2012; Heikkinen et al., 2013; Zhang and Dai, 2008; Zhang et al., 2012; Xiao et al., 2019).

From the mathematical point of view, the reconstruction of the spectral data from colorimetric information can be defined as an underdetermined system of equations where there are infinite solutions, i.e., spectral variable that fit the independent colorimetric data. Usually, the minimum norm solution is used to select a unique solution. In color science world, such system can be interpreted as metamer pairs and shows that, there are several reflectance spectra that provide identical color and the effort in this respect is restricted to find the spectra with the minimum spectral deviation from the actual reflectance values. However, various optimization techniques have been applied to minimize the differences between the estimated and the actual reflectance spectra. The main concern of this article is to introduce two regression methods, named support vector regression (SVR) and kernel ridge regression (KRR) in the spectral reconstruction attempt where the colorimetric data are available. Results of methods are compared to

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Table 1
The RMS, GFC, and ΔE^*_{ab} values between the actual and reconstructed spectra obtained from different methods.

Method	count	RMS			GFC			ΔE^*_{ab}					
								A			F11		
		mean	max	Std	mean	min	Std	mean	max	Std	mean	max	Std
SVR	634	0.016	0.149	0.018	0.996	0.763	0.015	1.185	9.268	1.199	1.444	11.955	1.499
KRR		0.015	0.178	0.020	0.997	0.837	0.009	1.036	11.387	1.563	1.351	14.499	1.926
PCA		0.024	0.149	0.018	0.993	0.809	0.013	1.717	11.217	1.663	2.238	12.735	2.164

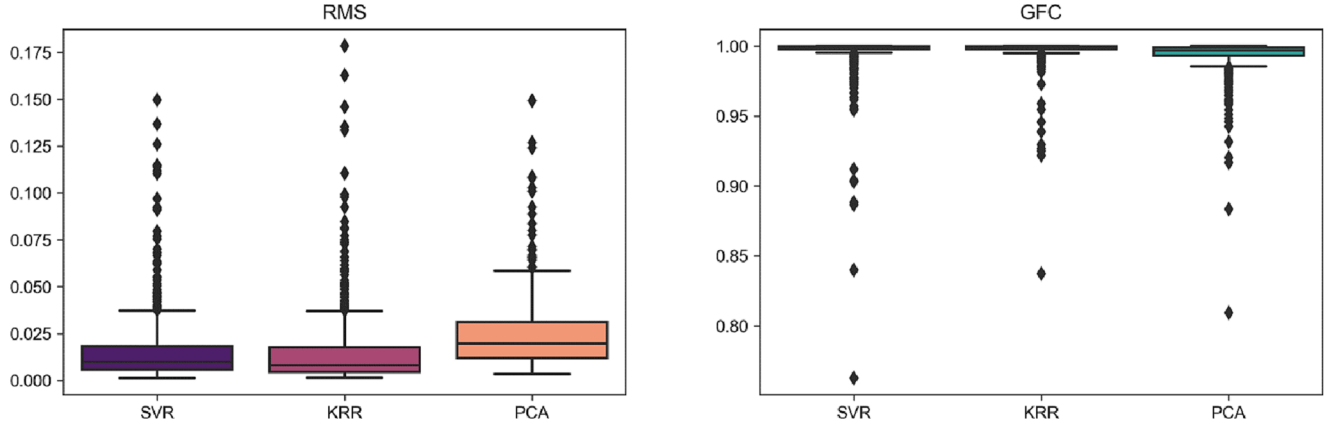

Fig. 1. Box plot diagram of the RMS and GFC values for SVR, KRR and PCA methods.

those obtained with conventional principal component analysis (PCA) technique.

2. Mathematical background

2.1. Support vector regression (SVR) method

While one tries to minimize the error between the actual and predicted values by classical regression approaches, the SVR estimates the best value within a certain threshold, i.e., the distance between the hyperplane and boundary line. This alteration makes the SVR a powerful and kernel-based regularization algorithm that allows the user to improve the error tolerance rate, both through an acceptable error margin and through adjusting the tolerance of the acceptable error rate. Indeed, it minimizes both the empirical risk and the confidence interval. The computational complexity of SVR does not depend on the size of the input space. It has been shown that SVR has excellent performance, especially for a low sample size with a high feature space dimension. In addition, it has excellent generalizability with high predictive accuracy. The SVR gives the flexibility to define how much error is acceptable in the model and find a suitable line (or hyperplane in higher dimension) that fits the data. In this method, with the help of a kernel trick, data is transferred from an n-dimensional space to the n + 1-dimensional space by maintaining relationships. The hyperplane that contains the most points is calculated in this space, and then some acceptable error constructs the decision boundaries.

In mathematical form, the model aims to minimize the function shown in Eq. (1):

$$minimize\ \frac{1}{2}||\beta||^2 + C\sum_{i=1}^{n}|\xi_i|,\ subject\ to ||\boldsymbol{R}_{train} - \widehat{\boldsymbol{r}}||_2^2 \leqslant \varepsilon + |\xi_i|, \tag{1}$$

Where, $\widehat{\boldsymbol{r}}$ is reconstructed reflectance calculated by:

$$\widehat{\boldsymbol{r}} = \boldsymbol{X}\boldsymbol{\beta} \tag{2}$$

Here, **X** is the matrix of independent variables, and $\boldsymbol{\beta}$ shows the vector of the parameters of the regression model. ε refers to margin error, and ξ is slack variables. For any value that falls outside of ε, its deviation from the margin can be denoted as ξ. C is an additional hyperparameter that defines the tolerance for points outside of ε. It should be noted that, in addition to the above parameters, there is also a gamma variable in the algorithms that is kernel coefficient. Gamma decides how much curvature there is at the decision boundary and higher gamma value indicates to more curvature (Vladimir, 2000; Drucker et al., 1997; Smola and Schölkopf, 2004).

2.2. . Kernel ridge regression (KRR) method

In multiple regression problems, determining the number of independent variables to be used in the model is a challenging decision. In fact, increasing the number of variables would lead to an overfitting problem and conversely, by decreasing of variables, the variance of the model can efficiently increase. One way to overcome these problems in the multiple regression analysis is to use the "ridge regression" model. Typically, an error function is used in the linear regression problem to minimize the "sum of squares of error". In ridge regression approach, by combining the function of the sum of squares of error and the amount of penalty related to the number of parameters, a new function is created, which is used to estimate the parameters of the regression model. Consequently, Eq. (3) shows the minimization function used by primal model (Ridge regression approach).

$$\begin{aligned} &\text{minimize} && \lambda||\boldsymbol{w}||^2 + \sum_{i=1}^{\ell}\xi_i^2, \\ &\text{subject to} && y_i - \langle \boldsymbol{w}\cdot\boldsymbol{x}_i\rangle = \xi_i, i = 1,\ldots,\ell, \end{aligned} \tag{3}$$

where, λ is called the penalty amount. In fact, it increases the residual sum of squares (RSS) value due to the increase in the number of parameters. Hence, the optimal value should be found by changing the value of λ that is followed by the estimation of model parameters and finally selecting the one which minimize the least square error.

Then, the Lagrangian model could be develop from Eq. (3):

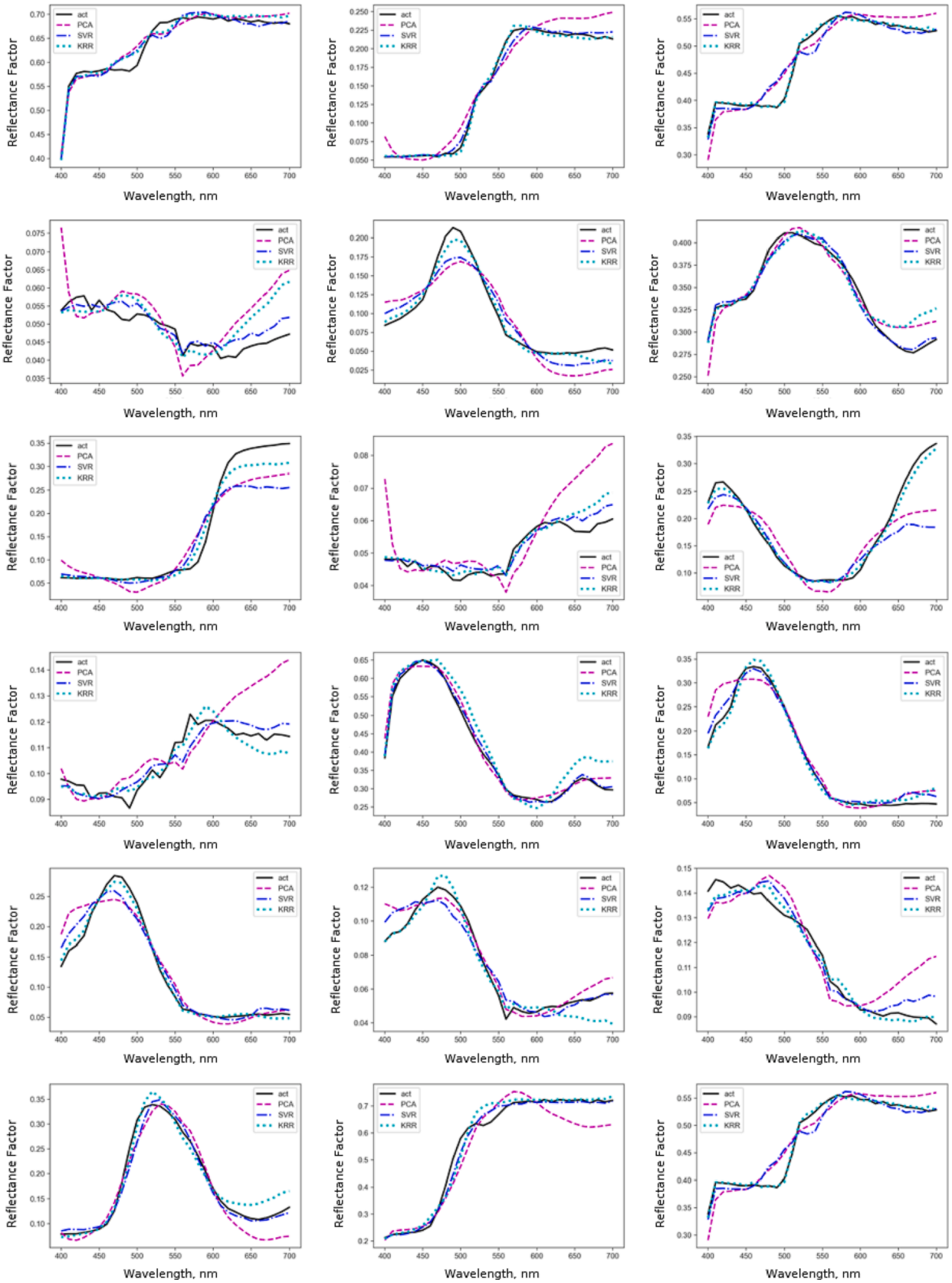

Fig. 2. The Actual and reconstructed spectra with different methods for 18 randomly selected samples.

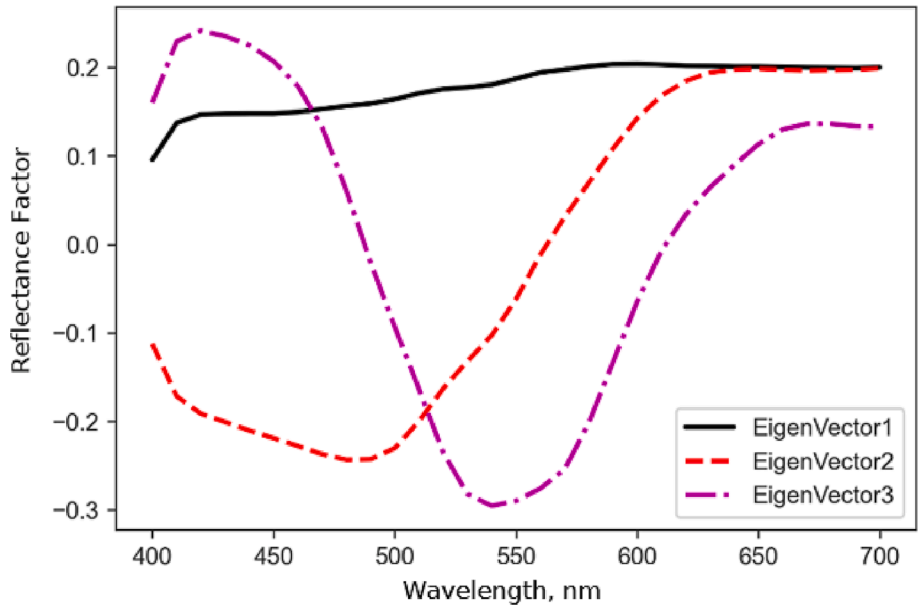

Fig. 3. The eigenvectors corresponding to the top three eigenvalues using odd samples of Munsell spectral dataset.

Table 2
Fitting and prediction times of SVR and KRR (mean ± std. dev. Of 7 runs, 10 loop each).

Method	Fitting time per loop	Prediction time per loop
SVR	2.05 s ± 113 ms	1.92 s ± 16.9
KRR	781 ms ± 76.4 ms	469 ms ± 84.1 ms

$$\text{minimize } L(\boldsymbol{w},\xi,\boldsymbol{\alpha}) = \lambda||\boldsymbol{w}||^2 + \sum_{i=1}^{\ell}\xi_i^2 + \sum_{i=1}^{\ell}\alpha_i(y_i - \langle \boldsymbol{w}\cdot\boldsymbol{x}_i\rangle - \xi_i)\ . \tag{4}$$

As a result of differentiation and static imposition, it is possible to show that:

$$\boldsymbol{w} = \frac{1}{2\lambda}\sum_{i=1}^{\ell}\alpha_i\boldsymbol{x}_i \text{ and } \xi_i = \frac{\alpha_i}{2}, \tag{5}$$

here, the dual problem arises by the resubstituting of the relations:

$$\text{maximize } W(\alpha) = \sum_{i=1}^{\ell} y_i\alpha_i - \frac{1}{4\lambda}\sum_{i,j=1}^{\ell}\alpha_i\alpha_j\langle \boldsymbol{x}_i\cdot\boldsymbol{x}_j\rangle - \frac{1}{4}\sum\alpha_i^2. \tag{6}$$

That can be represented by Eq. (7) in the vector form:

$$W(\boldsymbol{\alpha}) = \boldsymbol{y}'\boldsymbol{\alpha} - \frac{1}{4\lambda}\alpha'\mathbf{K}\boldsymbol{\alpha} - \frac{1}{4}\alpha'\boldsymbol{\alpha}, \tag{7}$$

where K denotes the Gram matrix $K_{ij} = \langle x_i \bullet x_j\rangle$, or in kernel-induced feature spaces is the kernel matrix $K_{ij} = k(x_i, x_j)$. Again, by differentiating with respect to α and imposing the stationarity condition:

$$-\frac{1}{2\lambda}\boldsymbol{K}\alpha - \frac{1}{2}\alpha + \boldsymbol{y} = 0 \rightarrow \boldsymbol{\alpha} = 2\lambda(\boldsymbol{K} + \lambda\boldsymbol{I})^{-1}\boldsymbol{y}. \tag{8}$$

And the corresponding regression function is given by Eq. (9).

$$f(\boldsymbol{x}) = \langle \boldsymbol{w}\cdot\boldsymbol{x}\rangle = \boldsymbol{y}'(\boldsymbol{K} + \lambda\boldsymbol{I})^{-1}\boldsymbol{k}, \tag{9}$$

which k is $k_i = \langle x_i \bullet x_j\rangle$, $i = 1,\ldots,\ell$.

As it is clear, the KRR is a simplified version of Support Vector Regression (Cristianini and Shawe-Taylor, 2000; Vovk et al., 2013).

Both KRR and SVR learn a nonlinear function by using a kernel trick. For example, both algorithms learn a linear function in reduced space through the kernel corresponding to a nonlinear function in the main space. Nevertheless, their difference is in the error function (margin versus epsilon-sensitive error). While the KRR fitting is typically faster for medium-sized datasets, the estimation step is longer than SVR.

3. Experimental procedure

The data studied in this work was the reflectance spectra of 1269 Munsell matte chips (Finland UoE). The collected reflectance spectra were first fixed in the range of 400 to 700 nm at 10 nm intervals. Samples of the dataset were divided into two odd and even groups to use them as training and testing sets, i.e., 635 specimens for learning and 634 samples for fitting and testing sequences.

The CIE XYZ tristimulus values of train and test samples were calculated under D65 standard illuminant and 1964 standard observer and used to fit models and make predictions. All computations were performed using the Python programming language. Sklearn library was used for KRR and SVR calculations, and the optimal hyperparameters for these two methods were selected using the Grid-search technique. In both SVR and KRR methodologies, the optimal kernel was radial basis function (RBF) kernel. It is necessary to clarify that, both KRR and SVR were constructed for a training set with a single output. It means that, models were trained for each wavelengths separately including all training data in the given wavelength. Consequently, the predictions were individually possible for each wavelength. More clearly, the visible spectrum, i.e. 400 to 700 nm, was divided in 31 equal narrow bandwidths and the model was trained 31 times and then, the prediction was made for 31 cases, independently.

Results of the employed methods, i.e., PCA, SVR, and KRR, were spectrally compared to actual spectral reflectances of the test dataset by using the root mean square (RMS) error and the goodness fit coefficient (GFC), which is the cosine of the angle between the actual and reconstructed spectra. For the colorimetric comparison, the CIE LAB color difference values under A and F11 light sources and 1964 standard observer were calculated to evaluate the performance of each method.

4. Result and discussions

Table 1 shows the reflectance reconstruction results of the test dataset for the employed methods in terms of RMS and GFC as well as ΔE^*_{ab} color difference values.

More details on RMS and GFC values are also shown in Fig. 1 in the

form of boxplot diagrams.

Results of Table 1 and Fig. 1 show that both SVR and KRR methods have provided significantly better recovery performances than PCA. They totally yield smaller RMS and ΔE^*_{ab} with higher GFC values. For a better demonstration of the results, the actual reflectance spectra of 18 randomly selected samples and the corresponding reconstructed spectra by the employed methods are also shown in Fig. 2.

As the plots of Fig. 2 show, the reconstructed spectra obtained from SVR and KRR do significantly differ from PCA reconstructed spectra and are apparently more accurate. The evidence is more evident for red and blue specimens that have relatively higher reflectance intensities in the short and long wavelength regions of the visible spectrum. The reason for this result can be interpreted from the spectral patterns of the extracted basic functions by the PCA that are shown in Fig. 3. As can be seen in the figure, the eigenvectors have slightly identical shapes in the range of 650 to 700 nm. Further, the color matching functions of standard observer show negligible spectral responses in this region. Therefore, any spectral differences of samples within two ends of visible spectrum are minimized in calculation of the XYZ colorimetric values.

However, the computational costs of SVR and KRR reconstruction methods should be considered in any evaluation, and it is a fact that the cost of both approaches are much higher than the PCA. Table 2 shows the computation times of proposed regression methods in the fitting and prediction stages.

As Table 2 shows, the KRR is faster than SVR in both fitting and prediction steps for the employed dataset. Nevertheless, as mentioned before, the computation period could change depending on the size of the chosen dataset.

5. Conclusion

Three different methodologies, i.e., SVR, KRR and PCA were used to reconstruct the reflectance spectra of colored surfaces from the corresponding CIE XYZ tristimulus values calculated under D65 standard illuminant and 1964 standard observer. The optimal hyperparameters of the SVR and KRR were chosen by the grid-search algorithm applied for reflectance reconstruction. RBF kernel was used for both kernel-based methods. Results were analyzed in terms of RMS and GFC and ΔE^*_{ab} values. It was found that the SVR and KRR methods have led to more accurate results than the PCA approach. Both regression methods totally achieved similar responses and can be successfully used in spectral reconstruction. However, their computation times were significantly higher compared to the PCA method. Based on the results of this study, it could be concluded that the SVR and KRR methods are suitable alternative approaches for reconstruction of spectral data from colorimetric information.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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