Generalized Inverse-Approach Model for Spectral-Signal Recovery

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***Abstract*— We have studied the transformation system of a spectral signal to the response of the system as a linear mapping from higher to lower dimensional space in order to look more closely at inverse-approach models. The problem of spectral-signal recovery from the response of a transformation system is generally stated on the basis of the generalized inverse-approach theorem, which provides a modular model for generating a spectral signal from a given response value. The controlling criteria, including the robustness of the inverse model to perturbations of the response caused by noise, and the condition number for matrix inversion, are proposed, together with the mean square error, so as to create an efficient model for spectral-signal recovery. The spectral-reflectance recovery and color correction of natural surface color are numerically investigated to appraise different illuminant-observer transformation matrices based on the proposed controlling criteria both in the absence and the presence of noise.**

***Index Terms*— Color, inverse problem, spectral analysis, spectral-signal reconstruction.**

I. Introduction

THE RECENT development of multispectral imaging systems together with an urgent need for a hyper-spectral data-acquisition system have given rise to extensive research in imaging science aimed at finding efficient ways of acquiring multispectral signals [1], [2]. Within this context, the over-sampling of hyperspectral signals as well as the inevitable noise involved in recording images demand an efficient process for image storage, communication and restoration without any loss of information. On the contrary, typical color-image acquisition devices record under-sampling spectral signals for each pixel. The spectral reconstruction of pixels is highly desirable in order to retrieve the colorimetric information of the image under any illumination conditions [3].

Manuscript received November 26, 2011; revised July 25, 2012; accepted August 24, 2012. Date of publication September 13, 2012; date of current version January 8, 2013. The associate editor coordinating the review of this manuscript and approving it for publication was Prof. Oscar C. Au.

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Digital Object Identifier 10.1109/TIP.2012.2218823

In 1964 Cohen analyzed the reflectance spectra of 433 chips in the Munsell Book and fitted a linear model to a set of spectra [4]. This considerable achievement formed the foundations of spectral reflectance recovery using linear models [5]–[7]. On the basis of linear models of basis functions of the spectral dataset [8], [9] a variety of methods were later developed for spectral recovery in the field of color science [10]–[14]. Spectral-based techniques have also been investigated with the intention of recovering the reflectance of surface colors from the sensor response of a digital camera [15], [16].

As far as imaging applications are concerned, Bayesian inference for inverse problems has been widely used as a far-reaching tool for image restoration [17], [18]. In the Bayesian inference model for inverse problems the posterior distribution is obtained by prior knowledge of the signal and noise. The Wiener filter restoration method, resulting from Bayes theorem, is a common technique for signal restoration, image reconstruction and communications problems [3], [17]–[20]. In 1995 Brainard suggested that Bayesian method might be suitable for spectral recovery from the RGB sensor responses [21]. Bayesian decision theory was also employed to deal with the problem of color constancy to compute the posterior distribution of the illuminants and recover the physical properties of the surfaces in the scene for a given set of sensor responses [22]. The Wiener filter-restoration approach as a solution for inverse problems in imaging science has been widely used for spectral-reflectance reconstruction from image-capturing sensor responses [23]–[28] and also for color correction methods [29]–[32].

To build a parametric inverse-approach model for spectral recovery or color correction, a modular model is created, the arguments of which can be set up to optimize the inverse model based on a preferred criterion. We first of all present here a theoretical background to introduce a transformation system together with the Moore-Penrose inverse approach and Bayes' method for inverse problems. Subsequently, in Section III, we introduce a theorem as a generalized approach for inverse problems in spectral-signal recovery from the response of a transformation system. The proposed theorem provides a general parametric form to generate mathematically a set of spectra given an individual response. The proposed theorem is extended to include the presence of noise as a perturbation of response in a transformation system. Since the optimum lighting condition for practical spectral recovery has always been a matter of great concern in color and imaging technology, in Section IV we investigate spectral-signal recovery from the response of a transformation system in order to develop the controlling criteria for making an efficient inverse model. The proposed controlling criteria are designed to evaluate in a practical way the transformation matrix for choosing the optimum transformation system in color and imaging technology. In Section V we develop the color-correction methods based on GIA, and finally we conduct a numerical experiment to test the proposed criteria for different illuminant-observer transformation matrices in order to obtain the optimum light source for classical spectral recovery and color correction.

II. Theoretical Background

It is very common to adopt the vector space approach to relate input and output for a mathematical model in color and imaging applications [3], [33], [34]. So let us take the following forward transformation system of signal to response to be:

$$\boldsymbol{c} = \mathbf{A}^T \boldsymbol{r} + \boldsymbol{\epsilon}, \tag{1}$$

where $\boldsymbol{r}$ is the $n \times 1$ vector of the spectral signal, $\mathbf{A}$ the $n \times p$ system transformation matrix, $\boldsymbol{\epsilon}$ the signal-independent additive noise of the system and $\boldsymbol{c}$ the $p \times 1$ response vector. In practice we encounter the problem of a considerable loss of information due to transforming from spectral n-dimensional signal space, $\Re^n$, to p-dimensional response space, $\Re^p$, where $p < n$. The difficulties attached to this information loss will emerge when we need to estimate the unknown signal, $\boldsymbol{r}$, from its system response, $\boldsymbol{c}$.

One simple way of estimating $\boldsymbol{r}$ is to use the Moore-Penrose generalized inverse matrix $(\mathbf{A}^T)^\dagger$ [35], which for an ideal noiseless system is

$$\hat{\boldsymbol{r}} = (\mathbf{A}^T)^\dagger \boldsymbol{c}. \tag{2}$$

Another way of estimating $\boldsymbol{r}$ is to use the Bayes theorem,

$$p(\boldsymbol{r}|\boldsymbol{c}) = \frac{p(\boldsymbol{c}|\boldsymbol{r})p(\boldsymbol{r})}{p(\boldsymbol{c})}, \tag{3}$$

in which $p(\boldsymbol{c}|\boldsymbol{r})$ and $p(\boldsymbol{r})$ are the likelihood and prior probability density functions respectively. Assuming Gaussian distribution, applying Eq. (3) to Eq. (1) would yield an analytical solution to the estimation of $\boldsymbol{r}$ given response $\boldsymbol{c}$ [17]. Translating our prior knowledge of the input signal $\boldsymbol{r}$ through prior probability distribution $\boldsymbol{r} \sim \mathcal{N}(\boldsymbol{\mu}_r, \Sigma_r)$ and assuming that the noise follows Gaussian distribution, $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\mu}_\epsilon, \Sigma_\epsilon)$, will result in the posterior probability distribution $p(\boldsymbol{r}|\boldsymbol{c}) = \mathcal{N}(\boldsymbol{\mu}_{r|c}, \Sigma_{r|c})$, where

$$\boldsymbol{\mu}_{r|c} = \Xi(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon - \mathbf{A}^T \boldsymbol{\mu}_r) + \boldsymbol{\mu}_r \tag{4}$$

$$\Sigma_{r|c} = \Sigma_r - \Xi \mathbf{A}^T \Sigma_r, \tag{5}$$

in which $\Xi = \Sigma_r \mathbf{A}(\mathbf{A}^T \Sigma_r \mathbf{A} + \Sigma_\epsilon)^{-1}$ is the Wiener estimation matrix [18]. The mean vector and covariance matrix are represented by $\boldsymbol{\mu}$ and Σ respectively. The estimation, $\hat{\boldsymbol{r}}$, of the signal, $\boldsymbol{r}$, given response $\boldsymbol{c}$, which minimizes the mean square error, $E\{\|\boldsymbol{r} - \hat{\boldsymbol{r}}\|^2\}$, is the mean vector $\boldsymbol{\mu}_{r|c}$. If, based on Eq. (3), the closed-form of the analytical solution is not available for an individual *a priori* and likelihood distributions; the estimation $\hat{\boldsymbol{r}}$ is the maximum *a posteriori*

$$\hat{\boldsymbol{r}} = \underset{\boldsymbol{r}}{argmax}\{p(\boldsymbol{c}|\boldsymbol{r})p(\boldsymbol{r})\}, \tag{6}$$

which is the most probable estimation of $\boldsymbol{r}$ given response $\boldsymbol{c}$ [17].

III. Generalized Inverse-Approach Theorem

In many applications where complete information is available about the transformation matrix, $\mathbf{A}$, it would be desirable to estimate $\hat{\boldsymbol{r}}$ efficiently from the response $\boldsymbol{c}$. The concept of the *Generalized Spectral-Decomposition Theorem* (GSD) was introduced for the metameric decomposition of spectral stimuli [36]. We intend to present here a *Generalized Inverse-Approach Theorem* (GIA) based on the same concept of GSD as well as its extension to include the presence of noise. From Appendix (A) we can estimate the signal $\hat{\boldsymbol{r}}_c$, given response $\boldsymbol{c}$. Now a general theorem is presented for the inverse problem that enables us to estimate the distribution $p(\boldsymbol{r}|\boldsymbol{c}) = \mathcal{N}(\hat{\boldsymbol{\mu}}_r, \hat{\Sigma}_r)$.

Theorem 1: Let $\boldsymbol{r}$ be a spectral signal that follows a Gaussian distribution, $\boldsymbol{r} \sim \mathcal{N}(\boldsymbol{\mu}_r, \Sigma_r)$, and $\boldsymbol{c} = \mathbf{A}^T \boldsymbol{r}$ an ideal noiseless system of signal $\boldsymbol{r}$ to response $\boldsymbol{c}$ transformation, which maps the higher n-dimensional signal space $\Re^n$ to the lower p-dimensional response space $\Re^p$. Let $\mathbf{S} = \mathbf{U\Omega U}^T\mathbf{V}(\mathbf{A}^T\mathbf{U\Omega U}^T\mathbf{V})^{-1}$ be a specified $n \times p$ matrix in which $\mathbf{U}$ and $\mathbf{V}$ are $n \times q$ and $n \times p$ matrices, respectively, where $p \le q \le n$. If the columns of the matrices $\mathbf{U}$ and $\mathbf{V}$ are specific, linearly independent, spectral basis vectors, and $\boldsymbol{\Omega}$ is a $q \times q$ individual real diagonal matrix, then $\hat{\boldsymbol{r}} = \boldsymbol{r}^c + \boldsymbol{r}^o$, with the constant fundamental signal

$$\boldsymbol{r}^c = \mathbf{S}\boldsymbol{c}, \tag{7}$$

and the nullspace

$$\boldsymbol{r}^o = \boldsymbol{r} - \mathbf{S}\mathbf{A}^T \boldsymbol{r} \tag{8}$$

of the transformation system, in which $\mathbf{H} = \mathbf{S}\mathbf{A}^T$ is an idempotent matrix, provides a spectral signal $\hat{\boldsymbol{r}}$ with the mean vector

$$\hat{\boldsymbol{\mu}}_r = \mathbf{S}(\boldsymbol{c} - \mathbf{A}^T \boldsymbol{\mu}_r) + \boldsymbol{\mu}_r \tag{9}$$

and covariance matrix

$$\hat{\Sigma}_r = (\mathbf{I} - \mathbf{H})\Sigma_r(\mathbf{I} - \mathbf{H})^T \tag{10}$$

so that $\mathbf{A}^T\hat{\boldsymbol{r}} = \boldsymbol{c}$ for the response $\boldsymbol{c}$ of the transformation system.

Proof: From Appendix (A), $\boldsymbol{r}^c = \mathbf{S}\boldsymbol{c}$ is an estimate of $\boldsymbol{r}$ with a noiseless response, $\boldsymbol{c}$. If the spectral signal $\hat{\boldsymbol{r}}$ provides the same response $\boldsymbol{c}$, then multiplying the signal $\hat{\boldsymbol{r}}$ by the transformation matrix $\mathbf{A}^T$ should result in the same response $\boldsymbol{c}$:

$$\mathbf{A}^T\hat{\boldsymbol{r}} = \mathbf{A}^T\boldsymbol{r}^c + \mathbf{A}^T\boldsymbol{r}^o. \tag{11}$$

The substitution of $\boldsymbol{r}^c$ and $\boldsymbol{r}^o$ from Eqs (7) and (8) into Eq. (11) gives:

$$\begin{aligned}\mathbf{A}^T\hat{\boldsymbol{r}} &= \mathbf{A}^T\mathbf{S}\boldsymbol{c} + \mathbf{A}^T(\boldsymbol{r} - \mathbf{S}\mathbf{A}^T\boldsymbol{r}) \\ &= \boldsymbol{c} + \mathbf{A}^T\boldsymbol{r} - \mathbf{A}^T\mathbf{S}\mathbf{A}^T\boldsymbol{r} \\ &= \boldsymbol{c} + \mathbf{A}^T\boldsymbol{r} - \mathbf{A}^T\boldsymbol{r} \\ &= \boldsymbol{c}. \end{aligned} \tag{12}$$

If $\boldsymbol{r}^o$ provides a signal of the nullspace $null(\mathbf{A}^T) := \{\boldsymbol{r}|\mathbf{A}^T\boldsymbol{r} = \mathbf{0}\}$ of the transformation system, then $\mathbf{A}^T\boldsymbol{r}^o = \mathbf{0}$. Considering Eq. (8):

$$\begin{aligned}\mathbf{A}^T\boldsymbol{r}^o &= \mathbf{A}^T(\boldsymbol{r} - \mathbf{S}\mathbf{A}^T\boldsymbol{r}) \\ &= \mathbf{A}^T\boldsymbol{r} - \mathbf{A}^T\mathbf{S}\mathbf{A}^T\boldsymbol{r} \\ &= \mathbf{A}^T\boldsymbol{r} - \mathbf{A}^T\boldsymbol{r} \\ &= \mathbf{0}. \end{aligned} \tag{13}$$

It can also be shown that for a scalar value γ, $\mathbf{A}^T(\gamma\,\boldsymbol{r}^o) = \mathbf{0}$. Furthermore, since $\mathbf{HH} = \mathbf{H}$ then $\mathbf{H} = \mathbf{S}\mathbf{A}^T$ is idempotent. Therefore, from Eqs (7) and (8), we can write:

$$\hat{\boldsymbol{r}} = \mathbf{S}\boldsymbol{c} + (\mathbf{I} - \mathbf{S}\mathbf{A}^T)\boldsymbol{r}. \tag{14}$$

Since $\boldsymbol{c}$ is a given deterministic vector, we get:

$$\begin{aligned}\hat{\boldsymbol{\mu}}_r &= \mathbf{S}\boldsymbol{c} + (\mathbf{I} - \mathbf{S}\mathbf{A}^T)\boldsymbol{\mu}_r \\ &= \mathbf{S}(\boldsymbol{c} - \mathbf{A}^T\boldsymbol{\mu}_r) + \boldsymbol{\mu}_r\end{aligned} \tag{15}$$

and

$$\begin{aligned}\hat{\Sigma}_r &= (\mathbf{I} - \mathbf{S}\mathbf{A}^T)\Sigma_r(\mathbf{I} - \mathbf{S}\mathbf{A}^T)^T \\ &= (\mathbf{I} - \mathbf{H})\Sigma_r(\mathbf{I} - \mathbf{H})^T.\end{aligned} \tag{16}$$

In the presence of noise $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\mu}_\epsilon, \Sigma_\epsilon)$ we could construct the following equation from Eq. (A.13) of Appendix (A),

$$\hat{\boldsymbol{\mu}}_r = \mathbf{S}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon - \mathbf{A}^T\boldsymbol{\mu}_r) + \boldsymbol{\mu}_r \tag{17}$$

and the covariance matrix $\hat{\Sigma}_r = (\mathbf{I} - \mathbf{S}\mathbf{A}^T)\Sigma_r(\mathbf{I} - \mathbf{S}\mathbf{A}^T)^T$, where,

$$\mathbf{S} = \mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon)^{-\mathbf{1}} \tag{18}$$

on the presumption that,

$$\tau = \| \, (\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-1}\Sigma_\epsilon) \, \| < 1, \tag{19}$$

so that $(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon)$ is invertible [37].

The proposed theorem would provide a parametric tool that enables us to create the modular convex subset $\hat{\mathcal{R}}^n(\boldsymbol{\Omega}) := \{\hat{\boldsymbol{r}}_i\}_{i=1}^m$ from the set of spectral signals, $\mathcal{R}^n := \{\boldsymbol{r}_i\}_{i=1}^m$, for a given response, $\boldsymbol{c}$, and specified matrices, $\mathbf{U}$ and $\mathbf{V}$. The properties of the subset thus created, $\hat{\mathcal{R}}^n(\boldsymbol{\Omega})$, will change depending on the input parameters and matrices chosen. In practical situation of the spectral recovery where $p < q \leq n$, we encounter the problem of information loss due to the transformation from higher dimensional spectral space to lower dimensional response space. Also, the spectral reflectance, $\boldsymbol{r}$, is unknown and we are not aware of the vector of residuals error, $\boldsymbol{e}$, in Eq.(A.3). As the result, the diagonal elements, ω_j, of the matrix $\boldsymbol{\Omega}$ are unknown. Therefore, the elements ω_j of the diagonal matrix $\boldsymbol{\Omega}$ as well as the matrices $\mathbf{U}$ and $\mathbf{V}$ should be optimized to efficiently recover the unknown $n \times 1$ spectral signal, $\boldsymbol{r}$, from the $p \times 1$ response vector, $\boldsymbol{c}$.

IV. Spectral Signal Recovery

The proposed GIA could be used to recover spectra from the response of a system. Taking the mean vector, $\hat{\boldsymbol{\mu}}_r$, as the estimated signal, $\hat{\boldsymbol{r}}$, we can write the following equation for spectral approximation from the response $\boldsymbol{c}$:

$$\begin{aligned}\hat{\boldsymbol{r}} &= \mathbf{S}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon - \mathbf{A}^T\boldsymbol{\mu}_r) + \boldsymbol{\mu}_r \\ &= \mathbf{S}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon) + (\mathbf{I} - \mathbf{H})\boldsymbol{\mu}_r.\end{aligned} \tag{20}$$

The two important special cases of GIA in terms of the aim of the inverse problem are:

1) An approach based on the Moore-Penrose generalized inverse matrix when $\boldsymbol{\Omega}$ is an $n \times n$ diagonal matrix equal to identity and $\mathbf{V} = \mathbf{A}$.
2) The Wiener inverse approach when $\boldsymbol{\Omega}$ is an $n \times n$ diagonal matrix, the diagonal elements of which are the descending-ordered eigenvalues of the covariance matrix Σ_r and $\mathbf{V} = \mathbf{A}$.

The proposed GIA was introduced based on the assumption of Gaussian distribution for spectral signal $\boldsymbol{r}$. The normal probability distribution can be roughly assumed for *a priori* and likelihood distributions that leads to a Gaussian posterior distribution. Nonetheless, the assumption of a Gaussian distribution of natural object spectra was argued in a paper by Attewell and Baddeley [38] where a beta-distribution or mixture of normal distributions for natural reflectance spectra were proposed. GIA holds true theoretically for the chosen parameters, yet optimizing the input arguments of GIA to construct an efficient model is required for practical applications in imaging and color science. The arguments of the model can be optimized to achieve a specific criterion, e.g. minimax of the estimation error. In this special case, in order to obtain the minimum of the maximum spectral estimation error using the training spectral dataset, the diagonal elements ω_j of the matrix $\boldsymbol{\Omega}$ can be optimized by,

$$\boldsymbol{\Omega}^* = \underset{\omega_j \neq 0}{argmin}\left\{max[\|\boldsymbol{r} - \hat{\boldsymbol{r}}(\boldsymbol{\Omega})\|^2]\right\}, \tag{21}$$

where $\hat{\boldsymbol{r}}$ is estimated using Eq. (20). In the following sections, two criteria are developed to control the system to create an efficient inverse model.

A. Mean Square Error of the Spectral Estimation

On the basis of Eq. (20) it can easily be proved that the mean square error, $E\{\|\boldsymbol{r} - \hat{\boldsymbol{r}}\|^2\}$, for the estimation of $\hat{\boldsymbol{r}}$ from $\boldsymbol{c}$ can be measured by:

$$\begin{aligned}\zeta &= E\left\{(\boldsymbol{r} - \mathbf{H}\boldsymbol{r})^T(\boldsymbol{r} - \mathbf{H}\boldsymbol{r})\right\} \\ &= \mathrm{tr}\left\{E[(\mathbf{I} - \mathbf{H})\boldsymbol{r}\boldsymbol{r}^T(\mathbf{I} - \mathbf{H})^T]\right\} \\ &= \mathrm{tr}\left\{(\mathbf{I} - \mathbf{H})\Sigma_r(\mathbf{I} - \mathbf{H})^T\right\} \\ &= \mathrm{tr}\{\hat{\Sigma}_r\}\end{aligned} \tag{22}$$

where $\mathrm{tr}\{\cdot\}$ is the *trace* operator. Rewriting Eq. (20) as the estimated signal, $\hat{\boldsymbol{r}}$, we have:

$$\hat{\boldsymbol{r}} = \boldsymbol{r}^c + (\mathbf{I} - \mathbf{H})\boldsymbol{\mu}_r - \mathbf{S}\boldsymbol{\mu}_\epsilon, \tag{23}$$

in which $\boldsymbol{r}^c$ is in fact the row estimation of the signal $\boldsymbol{r}$, $(\mathbf{I}-\mathbf{H})$ $\boldsymbol{\mu}_r$ is the average of the nullspace $\mathcal{R}_o^n$ of the transformation and $\mathbf{S}\boldsymbol{\mu}_\epsilon$ is an estimation of the spectral perturbation caused by noise $\boldsymbol{\epsilon}$. The term $(\mathbf{I} - \mathbf{H})\boldsymbol{\mu}_r$ is in fact the average of our unawareness about the signal being recovered, which is added to $\boldsymbol{r}^c$ just to compensate for the information loss caused by the transformation $\Re^n \mapsto \Re^p$ [36]. The covariance matrix $\hat{\Sigma}_r$ of the convex subset $\hat{\mathcal{R}}^n$ is equal to the covariance of $\mathcal{R}_o^n$. We may conclude that the amount of information loss might correspond to the extension of the nullspace, $\mathcal{R}_o^n$, or convex subset, $\hat{\mathcal{R}}^n$, which could be evaluated by the covariance matrix, $\hat{\Sigma}_r$. Therefore, we could measure information loss as a quantity related to the volume of the spectral space created by the convex subset, $\hat{\mathcal{R}}^n$. According to the information theory, the entropy of a Gaussian distribution is measured as a function of the product of eigenvalues of the corresponding covariance matrix. Furthermore, the continuous probability function, with higher differential entropy, contains more information in volume [39], [40]. Bearing in mind that the covariance, $\hat{\Sigma}_r$, is a positive definite matrix, the criterion for measuring the amount of information loss caused by the projection of Eq. (1) from the n-dimensional signal space, $\Re^n$, to the p-dimensional response space, $\Re^p$, could be numerically evaluated by the summation of the eigenvalues of $\hat{\Sigma}_r$, as presented in Eq. (22). Thus it is comprehensible that less information loss due to the transformation $\Re^n \mapsto \Re^p$ would provide more precise estimation, $\hat{\boldsymbol{r}}$, for the signal $\boldsymbol{r}$ given the response $\boldsymbol{c}$. It should be noted that, however, MSE is one of the most widely used criteria to control the inverse model, the sensitivity of the system to the noise perturbation is also of important consideration in the presence of noise, that should be taken into account together with MSE.

B. Perturbation of the System

In practical applications of imaging technology, the response is recorded by a noisy sensor device and the noise of the system may have a significant effect on the result of spectral recovery. Shimano [41] optimized a set of Gaussian-shaped spectral sensitivities based on a colorimetric evaluation in the presence of noise, in order to increase the robustness of the model to noise. He discussed that the robustness to noise decreases with an increase in the number of sensors at low SNRs, resulting in decreasing the performance of capturing the colorimetric information. In another research [26], he also proposed a model for estimating the system noise variance that can be used, together with the autocorrelation matrix, to effectively recover the spectral data [42]. In Appendix (A) it can be seen that the condition number of the matrix, $\mathbf{A}^T\mathbf{U}\Omega\mathbf{U}^T\mathbf{V}$, plays a crucial role in the estimation of $\hat{\boldsymbol{r}}$, and so a smaller condition number, $cond(\mathbf{A}^T\mathbf{U}\Omega\mathbf{U}^T\mathbf{V})$, may limit the relative error in estimating $\hat{\boldsymbol{r}}$ due to noise $\boldsymbol{\epsilon}$. This result is in agreement with previous finding that the inverse model is more sensitive to noise when the condition number is high [43].

In Eq. (20), it can be seen that any deviation of $\boldsymbol{c}$ results in a concomitant deviation in the approximated spectral signal, $\hat{\boldsymbol{r}}$. Therefore, it is preferable to have a model that is robust to the noise of the system so that the recovered signal $\hat{\boldsymbol{r}}$ deviates as little as possible while $\boldsymbol{c}$ is perturbed by the inevitable noise of the recording device. The derivative of the recovered signal $\hat{\boldsymbol{r}}$ of Eq. (20) with respect to response $\boldsymbol{c}$,

$$\frac{\partial \hat{\boldsymbol{r}}}{\partial \boldsymbol{c}} = \mathbf{S}, \tag{24}$$

provides the rate of perturbation of the spectrum, $\hat{\boldsymbol{r}}$, with a small deviation of $\boldsymbol{c}$ due to the noise of the system, $\boldsymbol{\epsilon}$. Therefore the magnitude of the perturbation rate of Eq. (24) can be considered as being a criterion for the evaluation of the robustness of the recovered spectral signal to the perturbation caused by the noise of the system, as follows:

$$\eta = \| \mathbf{S} \|, \tag{25}$$

where η measures the sensitivity of $\hat{\boldsymbol{r}}$ to perturbations in $\boldsymbol{c}$.

V. Color Correction

Color correction is the mapping procedure from a device-dependent response space such as sensor response to a device-independent color space such as CIEXYZ or CIELAB [30], [32]. Color correction methods and spectral approximation techniques both generally follow the same aim of estimating the colorimetric information of a color sample from the recorded response, $\boldsymbol{c}$, under many different viewing conditions. Let us suppose that $\mathbf{L} = [\varpi_i \mathcal{L}_i], i = 1, \ldots, K$ represents the $3K \times n$ matrix including K matrices $\mathcal{L}_i$, which is the $3 \times n$ CIE standard illuminant-observer matrix of mapping the reflectance spectra to the CIEXYZ color space. The scalar value ϖ_i represents the weighting factor corresponding to the viewing condition $\mathcal{L}_i$ proportional to its relative importance. Multiplication of Eq. (20) by $\mathbf{L}$ will result in the color correction model,

$$\begin{aligned} \boldsymbol{t} &= \mathbf{LS}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon - \mathbf{A}^T\boldsymbol{\mu}_r) + \mathbf{L}\boldsymbol{\mu}_r \\ &= \mathbf{LS}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon) + \mathbf{L}(\mathbf{I} - \mathbf{H})\boldsymbol{\mu}_r, \end{aligned} \tag{26}$$

which transforms the response vector $\boldsymbol{c}$ to the vector of tristimulus values $\boldsymbol{t} = \mathbf{L}\hat{\boldsymbol{r}}$, where

$$\zeta_c = \mathrm{tr}\{\ \mathbf{L}(\mathbf{I} - \mathbf{H})\Sigma_r(\mathbf{I} - \mathbf{H})^T\mathbf{L}^T\} \tag{27}$$

and

$$\eta_c = \| \mathbf{LS} \| \tag{28}$$

are respectively MSE and the perturbation sensitivity of the color-correction model of Eq. (26).

VI. Corollary

From Appendix (B) it has been shown that for an ideal noiseless system, given that $\mathbf{U}\Omega\mathbf{U}^T = \Sigma_r$ and $\mathbf{V} = \mathbf{A}$, the MSE value, ζ, is minimized. If $\mathbf{V} = \mathbf{A}$ and Ω is a diagonal matrix, the diagonal elements of which are equal to the decreasingly ordered eigenvalues of Σ_r then GIA would invert to the special case of the Wiener inverse model, meaning that amongst all possible special cases of GIA, whether it is applied in spectral space [10], [44] or principal-component space [45], [46], the Wiener inverse method would provide the minimum MSE for a noiseless system.

Vrhel and Trussel [30] proposed an interesting method to design the optimum filters for color correction in the absence of noise. On the basis of their elaborate idea, we have been able to design the optimum transformation matrix **A** to obtain the minimum MSE for signal recovery from the response of the noiseless transformation system. According to Appendix (C), if $\mathbf{U\Omega U}^T = \Sigma_r$ and $\mathbf{V} = \mathbf{A}$, the value ζ of a noiseless system is confined within the interval $[\xi_{min}, \xi_{max}]$. To obtain the lowest possible value of ξ_{min} for the MSE value ζ with regard to the matrix **A**, the transformation matrix **A** should preferably be designed on the basis of any individuals $\mathbf{A}^* \in \mathcal{A}$ where:

$$\mathcal{A} := \{\mathbf{A}|\mathbf{A} = \Sigma_r^{-1/2}\mathbf{Q}^*\mathbf{Y}, \mathbf{Y} \in \mathcal{Y}_p\}, \tag{29}$$

in which the columns of matrix $\mathbf{Q}^*$ are the p eigenvectors associated with the p largest eigenvalues of the matrix Σ_r and $\mathcal{Y}_p$ denotes the set of $p \times p$ non-singular matrices, **Y**.

It has been discussed in Appendix (A) that in the presence of noise, the condition number of the matrix $\mathbf{A}^T\mathbf{U\Omega U}^T\mathbf{V}$, should be small to decrease the effect of noise on the estimation of spectrum, $\boldsymbol{r}^c$. This is in convincing agreement with Shimano's findings [41]. Let's consider the special case of Wiener inverse model. Then, the singular values - and particularly the smaller ones - of the matrix $\mathbf{A}^T\mathbf{U\Omega}^{\mathbf{1/2}}$ should be maximized to increase the robustness of the model to noise [26], [41], [47]. The singular values of the matrix $\mathbf{A}^T\mathbf{U\Omega}^{\mathbf{1/2}}$ are equal to the square root of the eigenvalues of the matrix $\mathbf{A}^T\mathbf{U\Omega U}^T\mathbf{A}$, the condition number of which can be calculated by Eq. (A.14). Therefore, when the smallest singular value of the matrix $\mathbf{A}^T\mathbf{U\Omega}^{\mathbf{1/2}}$ gets closer to the largest one, the condition number of the matrix $\mathbf{A}^T\mathbf{U\Omega U}^T\mathbf{A}$ decreases, getting closer to one. In the present paper, we proposed the sensitivity of inverse-model to the noise perturbation based on Eq. (25), however, the sum of the squared singular values of the matrix **S** was proposed by Hironaga and Shimano to evaluate the robustness of the system to noise [48]. In the presence of noise $\boldsymbol{\epsilon}$, not only is the MSE value ζ of crucial concern [31] but also the robustness of the recovered spectral signal, $\hat{\boldsymbol{r}}$, to the perturbations in $\boldsymbol{c}$ due to the noise of the system, this latter being calculated according to the value η of Eq. (25). Thus, the optimum transformation matrix is that which provides the minimum MSE value, ζ, and simultaneously as low a value as possible for the sensitivity, η, of $\hat{\boldsymbol{r}}$ to perturbations in $\boldsymbol{c}$.

VII. Numerical Experiment

We undertook multispectral signal reconstruction of the reflecting specimens. The primary multispectral dataset included three sets of the reflectance collection spectrally measured from 400 to 700 (nm) with intervals of 10 (nm). The first set was the spectral data of 1269 chips in the Munsell Book of Color Matt Finish collection, measured at the University of Eastern Finland [49]. The second collection was the 1950 chips of the NCS Color Atlas [50], measured with the Datacolor 550TM spectrophotometer, and the third one consisted of 5574 samples of acrylic paint [9]. Therefore a total of 8793 reflectance spectra from natural color samples were available for the primary spectral dataset. In the following experiments, the total of 8793 spectral reflectances were used as the training dataset to construct the covariance matrix for inverse approach. Same dataset were also considered to be the trial set to test the inverse model.

TABLE I
Transformation Matrices With Different Matrix-Rank, p, That Are Created to Obtain the Minimum and Maximum MSE Values, ζ. the Table Also Shows the Percentage of the Positively Bounded Feasible Spectra Recovered From the Tristimulus Values Calculated by Using the Mentioned Transformation Matrix

p		ζ	Bounded $\hat{\boldsymbol{r}}$ (%)	Transformation Matrix
3	$\zeta_{\min}$	0.0894	96.5	A-2°
	$\zeta_{\max}$	0.1493	96.6	F5-10°
6	$\zeta_{\min}$	0.0128	99.5	F8-2°, A-2°
	$\zeta_{\max}$	0.0870	95.7	F10-10°, C-10°
9	$\zeta_{\min}$	0.0044	99.7	F7-10°, F5-10°, A-2°
	$\zeta_{\max}$	0.0585	96.0	F10-2°, F11-10°, F7-10°
12	$\zeta_{\min}$	0.0015	99.9	E-2°, F9-2°, F7-2°, A-10°,
	$\zeta_{\max}$	0.0378	98.4	F12-2°, F6-2°, F10-10°, F2-10°

A. Classical Spectral Recovery from Tristimulus Values

Recovery of reflectance spectra from the corresponding tristimulus values is of crucial importance in color science. In this part of the numerical experiment different transformation matrices were investigated using the value ζ, based on a noiseless transformation system. In the classical spectral-reconstruction methods [10], [12] the transformation matrix, **A**, is in fact the illuminant-observer matrix. In this part of the numerical analysis 16 illuminants, including equal energy (E), C, D65, A and 12 fluorescent light sources together with two sets of 10-degree 1964 and 2-degree 1931 standard observers, were used to create different illuminant-observer matrices, **A**, which is usually known as the spectral-power matrix. All the possible combinations of 32 illuminant-observer matrices available were used as the transformation matrix, **A**, to calculate the value of ζ. Thus the dimension p of each $n \times p$ transformation matrix **A**, created from the available illuminant-observer matrices, was a multiple of three. In Table 1, therefore, each row corresponding to a particular dimension represents the results obtained from the spectral recovery by the Wiener method using the transformation matrix, **A**, which provides minimum and maximum amounts of MSE values, ζ. The third column shows the percentage of feasible positive-bound spectra that can be recovered via the response of each transformation matrix. In each row the percentage of feasible spectra recovered via the response of the transformation matrix related to ζ_{min} is higher than that corresponding to ζ_{max}. It can be seen that the result for the best possible transformation matrix depends on the dimension p. Furthermore, the value of ζ decreases concomitantly with an increase in p. It is important to note that this numerical experiment was carried out to find the optimum illumination based on the optimum spectral performance, which does not essentially imply the optimum colorimetric performance. A model such as Eq. (26) may be constructed to find the minimum value of ζ_c that provides the optimum colorimetric performance under the chosen illumination, $\mathcal{L}_i$.

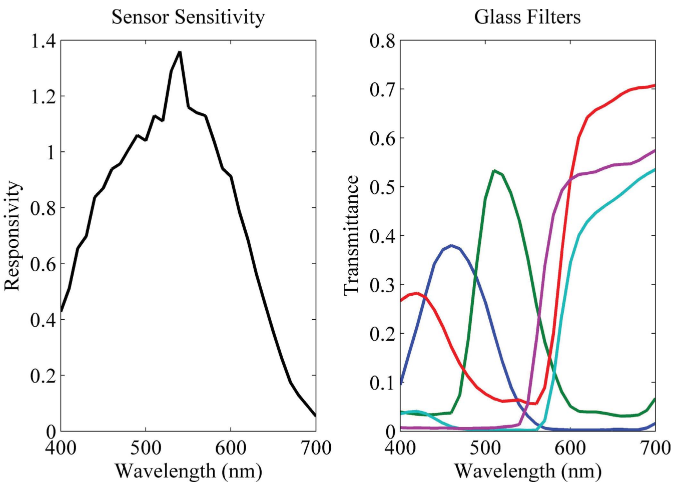

Fig. 1. Responsivity of the monochrome camera and transmittance of the five glass filters employed for recording response values.

B. Color Correction Using the Noisy Sensor Response

We used a monochrome 12-bit CCD camera from QImaging [51] together with 5 glass filters to record the 5×1 sensor responses, $\boldsymbol{c}$. Let us suppose that Λ is $n \times n$ the diagonal matrix, the diagonal elements of which are the spectral sensitivity of the sensor and $\mathbf{O}$ is $n \times p$ the matrix, the columns of which are the spectral transmittance factor of the glass filters. If the spectral-power distribution of the light source is written as a $n \times n$ diagonal matrix, $\mathbf{E}$, then the $n \times p$ transformation matrix, $\mathbf{A}$, is equal to $\Lambda\mathbf{EO}$. Because the 12-bit CCD sensor was used for image acquisition, each channel of the transformation matrix was normalized for the reflecting white sample so as to obtain the highest 12-bit response value, that for an ideal white sample is equal to 4095. Figure 1 represents the sensor sensitivity and the transmission spectra of the glass filters in the visible range of the spectrum. Noise $\boldsymbol{\epsilon}$ was presumed to follow normal distribution with $\boldsymbol{\mu}_\epsilon = \mathbf{0}$ and $\Sigma_\epsilon = \sigma_\epsilon^2 \mathbf{I}_5$, where the variances $\sigma_\epsilon^2 = 0.001$ and 0, corresponding to the SNRs of 30, and Inf dB respectively, were used in the experiment. In Appendix (A) we show that Eq. (19) should be satisfied in the presence of noise. Therefore, in the numerical experiment particular care has been taken to satisfy Eq. (19). However recording noiseless camera response is not practically possible by the real devices, the experiment was numerically carried out in the absence and presence of noise in order to evaluate the performance of color correction in both conditions using the perturbation sensitivity η_c together with MSE value ζ_c.

The numerical experiment was carried out to perform the color correction based on Eq. (26) in which the matrix $\mathbf{S}$ was created based on Eq. (18). The vectors of the tristimulus values, $\boldsymbol{t} = \mathbf{L}\hat{\boldsymbol{r}}$, of the 8,793 reflectance dataset from the responses of the chosen transformation matrices were estimated to test the color correction model. Matrix $\mathbf{L}$ was constructed by stacking the lighting matrices, $\mathcal{L}_i, i = 1, \ldots, 6$, with equal weighting factors, $\varpi_i = 1$, in which the matrices $\mathcal{L}_i$ were created by illuminants D65, A, F2, F5, F7 and F9 together with the 10-degree 1964 standard observer. The diagonal elements of $\mathbf{\Omega}$ were taken to be equal to the decreasingly ordered eigenvalues of the covariance matrix Σ_r and $\mathbf{V} = \Lambda\mathbf{EO}$. We then constructed the transformation matrices using the 16 available illuminants. Among the 16 possible transformation matrices, $\Lambda\mathbf{EO}$, constructed separately from the 16 available illuminants, the two which respectively led to the minimum values of MSE, ζ_c, and perturbation sensitivity, η_c, were chosen to create two different transformation systems. Then, the color correction was followed by numerical simulation of the recorded response values of the employed CCD under two selected illuminations, in the presence and absence of noise.

TABLE II
ANALYSIS OF THE COLOR CORRECTION PERFORMANCE WITH REGARD TO THE MSE VALUE, ζ_c, AND PERTURBATION SENSITIVITY, η_c, FOR TWO DIFFERENT TRANSFORMATION SYSTEMS, CALCULATED BY ΔE_{94}^* COLOR DIFFERENCE BOTH IN THE ABSENCE AND PRESENCE OF NOISE

SNR	No.	ζ_c	η_c	Min	Max	Mean	Median
Inf	1	1.4005	3.2090	0.4671	0.6796	0.5530	0.5412
	2	0.5886	9.9703	0.2987	0.4943	0.4301	0.4490
30	1	1.4006	3.1971	0.4819	0.6825	0.5648	0.5541
	2	0.6011	9.5328	0.5008	0.8061	0.6767	0.7086

The results of color correction conducted on the 8,793 samples to estimate their tristimulus values under illuminants D65, A, F2, F5, F7 and F9 from the response of the two chosen transformation systems are set out individually in Table II, in which the MSE value, ζ_c, and perturbation sensitivity, η_c, as well as the minimum, maximum, mean and median of the CIE94 color-difference, ΔE_{94}^*, obtained under the chosen illuminants and 10-degree 1964 standard observer, are all shown. The first transformation system showed minimum perturbation sensitivity, η_c, while its MSE was quite high, whereas the second one showed the minimum MSE value, ζ_c, but its perturbation sensitivity, η_c, was high. As Table II shows, in the absence of noise (SNR = Inf) the second transformation system with minimum MSE proved to be the better color correction model, the minimum, maximum, mean and median of ΔE_{94}^* of which were all smaller than those obtained with the first one. In the presence of noise (SNR = 30) the second transformation system, with a high perturbation sensitivity of $\eta_c = 9.5328$, gave rise to an unsatisfactory colorimetric performance in spite of its low MSE value of $\zeta_c = 0.6011$. It is very important to note that the second transformation, with a minimum MSE value, performed badly for color correction due to the fact that its perturbation sensitivity is high. It can be seen that in the presence of noise (SNR = 30) the first transformation, with a low perturbation sensitivity of $\eta_c = 3.1971$, performed best as far as colorimetric performance is concerned, even though its MSE value of $\zeta_c = 1.4006$ is high.

Figure 2 shows the average of ΔE_{94}^* between the estimated color coordinates of 8,793 samples and the real ones under the chosen illuminants for two different noise levels: SNR = 30 and SNR = Inf. It can be seen that the ΔE_{94}^* color differences for the second transformation system were generally lower that those obtained with the first transformation in the absence of noise (SNR = inf). In the presence of noise (SNR = 30) the

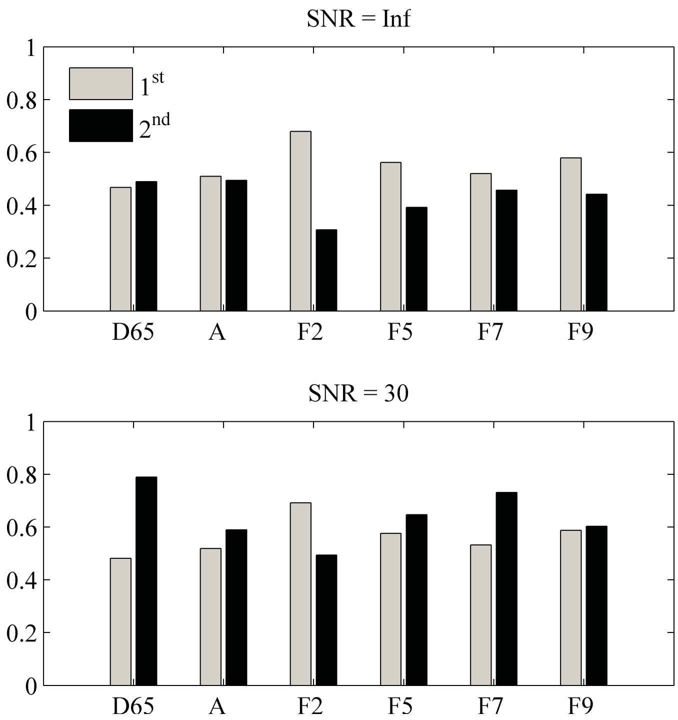

Fig. 2. Average of the ΔE^*_{94} color differences between the estimated color coordinates of 8793 samples and the real ones under illuminants D65, A, F2, F5, F7, and F9 for the two different transformation systems in the presence (SNR = 30) and absence (SNR = Inf) of noise. The first transformation system shows the lower perturbation sensitivity while the second one has the lower MSE value.

colorimetric performance of the second transformation system, with the higher perturbation sensitivity of $\eta_c = 9.5328$, decreased significantly. It is obvious that the color differences of the second transformation system under all illuminants except F2 are greater than that of the first transformation, while the colorimetric performance of the first one does not change to any considerable degree by imposing noise with SNR = 30 upon the system. It was discussed that the effect of the noise $\boldsymbol{\epsilon}$ in estimation of $\hat{\boldsymbol{r}}$ is decreased by the smaller condition number of the matrix, $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}$. In this context, smaller perturbation sensitivity corresponds to the smaller condition number that limits the effect of noise on the inverse model.

VIII. Conclusion

The generalized inverse-approach (GIA) theorem was formulated as a parametric model for generating a set of signals for the individual response of a transformation system and was established as a modular tool to facilitate the estimation of the distribution of the spectral signal $\boldsymbol{r}$ given response $\boldsymbol{c}$. An approach based on the Moore-Penrose generalized inverse matrix and also the Wiener inverse model are both special cases of the GIA theorem.

To construct an efficient inverse model we have investigated the controlling criteria: the mean square error (MSE), perturbation sensitivity of the system and condition number for matrix inversion. These criteria have enabled us to evaluate the transformation matrix, i.e. the lighting condition for spectral recovery and color correction in imaging applications. The performances of the proposed controlling criteria were assessed in practice via a numerical experiment for spectral approximation and color correction using noisy sensor response. The minimum MSE was also desirable for a noiseless system. Nevertheless, in the presence of noise, the robustness of the inverse model to perturbations due to the noise of the system plays a crucial role in creating an efficient inverse model for spectral-signal reconstruction. Therefore, an efficient inverse model should benefit from a low MSE value and simultaneously as low a perturbation sensitivity as possible in the presence of noise.

Appendix A

Let us now consider a particular $n \times 1$ signal, $\boldsymbol{r}$, that might be recovered by the linear combination of q basis functions, $\boldsymbol{u}_j$, by:

$$\boldsymbol{r} = \mathbf{U}\boldsymbol{\kappa} = \sum_{j=1}^{q} \kappa_j \boldsymbol{u}_j, \tag{A.1}$$

in which the $n \times q$ matrix, $\mathbf{U}$, is used to transform the spectral signal space, $\Re^n$, into basis component space, $\Re^q$, as:

$$\boldsymbol{\kappa} = \mathbf{U}^T\boldsymbol{r}, \tag{A.2}$$

where $\boldsymbol{\kappa}$ is a $q \times 1$ vector, the $\kappa_j = \boldsymbol{u}_j^T\boldsymbol{r}$ entries of which are the weights that uniquely identify the spectral signal, $\boldsymbol{r}$, as the coordinates in the component space, $\Re^q$. Now let us suppose that the $n \times 1$ signal, $\boldsymbol{r}$, can also be estimated approximately by the linear combination of p linearly independent vectors, $\boldsymbol{v}_k, k = 1, 2, \ldots, p \le q \le n$. Then, we have

$$\boldsymbol{r} = \mathbf{V}\boldsymbol{\alpha} + \boldsymbol{e}, \tag{A.3}$$

where the $n \times 1$ vectors $\boldsymbol{v}_k$ are the columns of $n \times p$ matrix $\mathbf{V}$ and $\boldsymbol{\alpha}$ is a $p \times 1$ vector, the α_k entries of which are the coefficients of linear summation and $\boldsymbol{e}$ is the $n \times 1$ vector of residual error. Since the component space, $\Re^q$, is spanned by $q \le n$ basis functions, the spectral signal $\boldsymbol{r}$ can be completely recovered by at most q linearly independent vectors, $\boldsymbol{v}_k$, and therefore, $p \ngtr q$. The j-th coordinate, κ_j, of $\boldsymbol{r}$ in the component space, $\Re^q$, can be calculated from Eq. (A.4) as follows:

$$\kappa_j = \boldsymbol{u}_j^T\boldsymbol{r} = \boldsymbol{u}_j^T\mathbf{V}\boldsymbol{\alpha} + \boldsymbol{u}_j^T\boldsymbol{e} = \omega_j\boldsymbol{u}_j^T\mathbf{V}\boldsymbol{\alpha} \tag{A.4}$$

in which,

$$\omega_j = \kappa_j(\kappa_j - \boldsymbol{u}_j^T\boldsymbol{e})^{-1} = \frac{\kappa_j}{\boldsymbol{u}_j^T\mathbf{V}\boldsymbol{\alpha}}. \tag{A.5}$$

Then Eq. (A.5) can be written in the matrix form of:

$$\boldsymbol{\kappa} = \boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}\boldsymbol{\alpha}, \tag{A.6}$$

where $\boldsymbol{\Omega}$ is a $q \times q$ diagonal matrix with diagonal elements ω_j, the rank of which is equal to q. Thus, with regard to Eqs (A.1) and (A.6), we can write:

$$\boldsymbol{r} = \mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}\boldsymbol{\alpha}. \tag{A.7}$$

Eq. (A.7) describes how the signal $\boldsymbol{r}$ can be completely recovered by the linear combination of p vectors in the columns of the $n \times p$ matrix $\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}$.

Suppose that we want to estimate the signal $\boldsymbol{r}^c \in \{\boldsymbol{r}|\mathbf{A}^T\boldsymbol{r} = \boldsymbol{c}\}$, where $\boldsymbol{c}$ is the $p \times 1$ vector of noiseless response of the system. Substituting $\boldsymbol{r}$ from Eq. (A.7) into the noiseless transformation system $\boldsymbol{c} = \mathbf{A}^T\boldsymbol{r}$, we get:

$$\boldsymbol{c} = \mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}\boldsymbol{\alpha}, \tag{A.8}$$

where the matrix $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}$ is a $p \times p$ non-singular full-rank matrix. Eq. (A.8) can then be solved for the $p \times 1$ vector of coefficients $\boldsymbol{\alpha}$ to yield:

$$\hat{\boldsymbol{\alpha}} = (\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-1}\boldsymbol{c}. \tag{A.9}$$

Substitution of the estimated coefficients vector $\hat{\boldsymbol{\alpha}}$ into Eq. (A.7) gives,

$$\boldsymbol{r}^c = \mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-\mathbf{1}}\boldsymbol{c}, \tag{A.10}$$

which is the estimation for $\boldsymbol{r}$ with noiseless response $\boldsymbol{c}$. It should be noted that if the vector of the residual error, $\boldsymbol{e}$, for estimating $\boldsymbol{r}$ based on Eq. (A.3) is known, the matrix, $\boldsymbol{\Omega}$, will be identified by Eq. (A.5) and then $\boldsymbol{r}^c = \boldsymbol{r}$, which is an exact estimation of $\boldsymbol{r}$ with noiseless response $\boldsymbol{c}$. In inverse problem of spectral estimation, the vector of residual error, $\boldsymbol{e}$, in Eq. (A.3) and therefore, the diagonal matrix, $\boldsymbol{\Omega}$, are practically unknown, unless $p = q$ and as the result, $\boldsymbol{e} = 0$. In practical situation of the spectral recovery from the response $\boldsymbol{c}$, where often $p < q \leq n$, we are not aware of the residual error, $\boldsymbol{e}$, and then, the diagonal elements ω_j are unknown.

In the presence of noise $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\mu}_\epsilon, \Sigma_\epsilon)$, the substitution of $\boldsymbol{r}$ from Eq. (A.7) into the noisy transformation system of Eq. (1) will result in:

$$\boldsymbol{c} = \mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}\boldsymbol{\alpha} + \boldsymbol{\epsilon}. \tag{A.11}$$

Like Eq. (A.8), Eq. (A.11) is a system of linear equations, but with uncertainty in the response data, $\boldsymbol{c}$, due to the presence of the noise, $\boldsymbol{\epsilon}$. An attempt to find a solution to Eq. (A.11) may include perturbation matrix due to the noise. Eq. (A.11) may be solved with uncertainty due to the presence of noise $\boldsymbol{\epsilon}$ to estimate $\hat{\boldsymbol{\alpha}}$ as follows [37]:

$$\hat{\boldsymbol{\alpha}} = (\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon)^{-1}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon), \tag{A.12}$$

where Σ_ϵ is supposed to be a perturbation matrix of $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}$ [52]. Introducing $\hat{\boldsymbol{\alpha}}$ from Eq. (A.12) into Eq. (A.7) results in:

$$\boldsymbol{r}^c = \mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon)^{-1}(\boldsymbol{c} - \boldsymbol{\mu}_\epsilon). \tag{A.13}$$

Since the matrix $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V}$ is supposed to be invertible, Σ_ϵ should be small enough for $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon$ also to be invertible. If the spectral radius of the matrix $(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-1}\Sigma_\epsilon$ is less than unitiy, the matrix $\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V} + \Sigma_\epsilon$ is invertible (see pp. 301–302, 335 of [37]). Thus to satisfy this condition, we take it that $\| (\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-1}\Sigma_\epsilon \| < 1$, where $\| \cdot \|$ is the matrix norm. The error of estimating $\hat{\boldsymbol{\alpha}}$ in the presence of noise $\boldsymbol{\epsilon}$ could contribute to estimating the signal $\boldsymbol{r}$. The upper bound on the relative error of estimating $\hat{\boldsymbol{\alpha}}$ could be described in terms of the condition number of matrix inversion with respect to the matrix norm that is defined for a matrix $\mathbf{X}$ as follows [37], [52],

$$cond(\mathbf{X}) = \| \mathbf{X}^{-1} \| \| \mathbf{X} \| = \left| \frac{\lambda_{max}(\mathbf{X})}{\lambda_{min}(\mathbf{X})} \right|, \tag{A.14}$$

where, λ is the eigenalue of the matrix $\mathbf{X}$. Therefore, the condition number, $cond(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})$, is of considerable importance in estimating $\boldsymbol{r}^c$ in the presence of noise $\boldsymbol{\epsilon}$. The system noise variance in the perturbation matrix Σ_ϵ can be practically estimated based on the interesting method proposed by Shimano [26].

Appendix B

Our aim in this appendix is to find the optimum matrix $\boldsymbol{\Omega}$ as the parameter of GIA that results in minimum information loss in order to be able to estimate the best spectral signal, $\boldsymbol{r}$, from the ideal noiseless system response, $\boldsymbol{c}$. For a noiseless transformation system $\boldsymbol{r}$ can be estimated from Eq. (9) by:

$$\hat{\boldsymbol{r}} = \mathbf{S}\boldsymbol{c} + (\mathbf{I} - \mathbf{H})\boldsymbol{\mu}_r. \tag{B.1}$$

On the basis of Eq. (23), MSE can be obtained by:

$$\zeta = \operatorname{tr}\{(\mathbf{I} - \mathbf{H})\Sigma_r(\mathbf{I} - \mathbf{H})^T\}. \tag{B.2}$$

To minimize ζ with respect to $\boldsymbol{\Omega}$, we take it that the convex subset $\hat{\mathcal{R}}^n(\boldsymbol{\Omega})$ is created by the specific matrices $\mathbf{U}$ and $\mathbf{V}$ and then begin with the derivative of ζ with respect to the diagonal elements ω_j of $\boldsymbol{\Omega}$ as follows:

$$\frac{\partial \zeta}{\partial \omega_j} = \frac{\partial \operatorname{tr}\{\hat{\Sigma}_r\}}{\partial \omega_j} = 0. \tag{B.3}$$

Performing some algebraic manipulation based on the rules of matrix derivatives [35], [53], [54], Eq. (B.3) can be written as:

$$\begin{aligned}\frac{\partial \zeta}{\partial \omega_j} &= \frac{\partial \operatorname{tr}\{\Sigma_r - \mathbf{H}\Sigma_r - \Sigma_r\mathbf{H}^T + \mathbf{H}\Sigma_r\mathbf{H}^T\}}{\partial \omega_j} \\ &= -2\operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\right\} + \operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\mathbf{H}^T + \mathbf{H}\Sigma_r\frac{\partial \mathbf{H}^T}{\partial \omega_j}\right\} \\ &= -2\operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\right\} + 2\operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\mathbf{H}^T\right\}.\end{aligned} \tag{B.4}$$

Then, we find that if

$$\operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\right\} = \operatorname{tr}\left\{\frac{\partial \mathbf{H}}{\partial \omega_j}\Sigma_r\mathbf{H}^T\right\}, \tag{B.5}$$

in which,

$$\frac{\partial \mathbf{H}}{\partial \omega_j} = (\mathbf{I} - \mathbf{H})\boldsymbol{u}_j\boldsymbol{u}_j^T\mathbf{V}(\mathbf{A}^T\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T\mathbf{V})^{-\mathbf{1}}\mathbf{A}^T \tag{B.6}$$

and thus the condition of Eq. (B.3) is satisfied. To satisfy the condition of Eq. (B.3) the $n \times 1$ vectors, $\boldsymbol{v}_k$, of the columns of matrix $\mathbf{V}$ should span the same range as that of the columns of $\mathbf{A}$. If $\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T = \Sigma_r$ and $\mathbf{A} = \mathbf{V}$ or the vectors $\boldsymbol{v}_k$ of the columns of $\mathbf{V}$ are equal to the orthogonalized columns of $\mathbf{A}$, then the condition of Eq. (B.3) is satisfied.

Appendix C

Let us suppose that an optimum GIA for a noiseless system is designed with $\mathbf{U}\boldsymbol{\Omega}\mathbf{U}^T = \Sigma_r$ and $\mathbf{A} = \mathbf{V}$. When finding the optimum transformation matrix, $\mathbf{A}$, the minimum MSE value, ζ, with respect to $\mathbf{A}$ is desirable for a noiseless system. Inserting $\mathbf{H} = \Sigma_r \mathbf{A}(\mathbf{A}^T \Sigma_r \mathbf{A})^{-1}\mathbf{A}^T$ into Eq. (B.2) results in:

$$\begin{aligned}\zeta &= \mathrm{tr}\{\Sigma_r - \Sigma_r \mathbf{A}(\mathbf{A}^T \Sigma_r \mathbf{A})^{-1}\mathbf{A}^T \Sigma_r\} \\ &= \mathrm{tr}\{\Sigma_r\} - \mathrm{tr}\{\Sigma_r \mathbf{A}(\mathbf{A}^T \Sigma_r \mathbf{A})^{-1}\mathbf{A}^T \Sigma_r\} \\ &= \mathrm{tr}\{\Sigma_r\} - \xi, \end{aligned} \tag{C.1}$$

where $0 < \xi = \mathrm{tr}\{\Sigma_r \mathbf{A}(\mathbf{A}^T \Sigma_r \mathbf{A})^{-1}\mathbf{A}^T \Sigma_r\} < \mathrm{tr}\{\Sigma_r\}$. Therefore, the bounds on the criterion of ζ will be obtained via the minimum and maximum values for ξ. To find the boundary of ζ let us consider the interesting method employed by Vrhel and Trussell [30]. If we define the $n \times p$ matrix $\mathbf{F} = \Sigma_r^{1/2}\mathbf{A}$, then:

$$\xi = \mathrm{tr}(\mathbf{Q}^T \Sigma_r \mathbf{Q}), \tag{C.2}$$

in which $\mathbf{F} = \mathbf{QY}$ is the result of the Gram-Schmidt orthogonalization process [55], in which $\mathbf{Q}$ is the $n \times p$ orthonormal matrix, and thus $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$ and $\mathbf{Y}$ is a $p \times p$ non-singular matrix. Thus the boundary values for ξ with regard to $\mathbf{Q}$ will be obtained as [37]:

$$\xi_{max} = \underset{\mathbf{Q}^T\mathbf{Q}=\mathbf{I}}{max} \left\{\mathrm{tr}(\mathbf{Q}^T \Sigma_r \mathbf{Q})\right\} = \sum_{i=1}^{p} \delta_i \tag{C.3}$$

$$\xi_{min} = \underset{\mathbf{Q}^T\mathbf{Q}=\mathbf{I}}{min} \left\{\mathrm{tr}(\mathbf{Q}^T \Sigma_r \mathbf{Q})\right\} = \sum_{i=p+1}^{n} \delta_i, \tag{C.4}$$

where $[\delta_1, \delta_2, \ldots, \delta_n]$ are the eigenvalues associated to the $n \times n$ matrix Σ_r and $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$. With regard to Eqs (C.3) and (C.4), Eq. (C.1) gives the bounds to the criterion MSE value, $\zeta \in [\xi_{min}, \xi_{max}]$.

ACKNOWLEDGMENT

The authors would like to thank the reviewers for their valuable comments and thoughtful suggestions, which helped to improve this paper.

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