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Principal Components Applied to Modeling: Dealing with the Mean Vector

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Abstract.

Principal components analysis is often used to fit a population of spectral reflectances by a mean vector plus a basis-function expansion about the mean. Certain color-technology applications (such as color correction) are much easier if the mean is absent. If the mean reflectance (or other spectral function) is a linear combination of the first few principal components (such as the first three), then a linear model can fit the original data without mentioning the mean vector in the model's formulation. This idea is worked out step by step, and a realistic example is presented.

Key Words: color constancy, color correction, linear model, principal components analysis, reflectance.

Introduction

In color science, so-called linear models are used to express the predictability among a population of functions, such as spectral reflectances. One source for empirical models is principal components (PC) analysis, a method to discover dependencies in data. Ideally, a linear model can become a tool for repeated use, independent of the data from which it was derived. Suppose that an analysis of object reflectances yields P orthonormal functions of wavelength, over domain $[\lambda_1, \lambda_2]$, written as $r_1(\lambda)$, $r_2(\lambda)$, $r_3(\lambda)$, $r_P(\lambda)$ or $|1\rangle$, $|2\rangle$, $|3\rangle$, ...$|P\rangle$. To say the functions are orthonormal means that

$$\int_{\lambda_1}^{\lambda_2} r_i r_j d\lambda = \langle i|j\rangle = \delta_{ij} , \tag{1}$$

where $\langle i|j\rangle$ is the inner product of the ith and jth basis functions, and δ_{ij} is the Kronecker delta, equal to 1 if $i=j$, and equal to 0 otherwise.

Orthonormal basis functions permit construction of a unity operator,

$$\mathbb{1} = \sum_{j=1}^{P} |j\rangle\langle j| \ , \tag{2}$$

with which a surface reflectance $|s\rangle$ may be modeled[1],

$$|s\rangle = \mathbb{1}|s\rangle \ . \tag{3}$$

If Q vectors are judged to suffice, and we truncate the sum at the Qth term, then

$$|s\rangle \approx |1\rangle\langle 1|s\rangle + |2\rangle\langle 2|s\rangle + ... + |Q\rangle\langle Q|s\rangle \ . \tag{4}$$

Complete brackets, such as $\langle 1|s\rangle$, denote inner products, meaning that they are scalars, namely the coefficients of the vectors $|1\rangle$, $|2\rangle$... $|Q\rangle$ in the expansion of this particular surface $|s\rangle$.

We assumed above that the PC analysis gives P orthonormal vectors. These are the full set that the analysis produces, or at least a large number that fit the original data well. A linear model may sacrifice accuracy to use only the first Q of the P functions that are available. For example, P might be 10, but Q might be 3. When the sum is truncated to give a less-than-perfect approximation, the unity operator becomes a projection operator. Whatever word is used, we keep the operator in the ket-bra form of Eqs. (2-4) to emphasize the role of orthonormal functions. For

now it suffices to say that a ket, $|j\rangle$, is a column matrix, and a bra, $\langle j|$, is its transpose, a row matrix. With this interpretation, Eq. (2) is an expression for Cohen's projection operator, Matrix R, supposing that $|1\rangle$, $|2\rangle$, and $|3\rangle$ are orthonormal color matching functions [1,2,3]. The projection operator is factored (broken apart) within the derivation of Eq. (4), showing a benefit of bras and kets. They emphasize the roles of vectors and inner products, and streamline some derivations. Given specific vectors, one could carry out the operations indicated in Eq. (2) to create a large square array of numbers, a valid "Matrix R," but that is not the goal here[1].

There is now a fly in the ointment. If the vectors $|j\rangle$ arise from principal components analysis, then Eqs. (2-4) are not in the correct form. The algorithm of principal components is:

1. Acquire a set of data vectors; for example, measure some M spectral reflectances $|s\rangle$.
2. Calculate the mean vector of the set. Call it $|0\rangle$.
3. Subtract that mean vector from each of the data vectors.
4. From the set of vectors thus adjusted, find the covariance matrix, then the eigenvalues and eigenvectors of that matrix.

The resulting vectors $|j\rangle$ are then not a basis for approximating vectors $|s\rangle$; they are a basis for "reduced vectors" ($|s\rangle - |0\rangle$), and Eq. (4) must be replaced by

$$|s\rangle \approx |0\rangle + |1\rangle\langle 1|(|s\rangle - |0\rangle) + ... + |Q\rangle\langle Q|(|s\rangle - |0\rangle) \quad . \tag{5}$$

Eq. (5) is inconvenient, especially if one would seek to write a unity operator. Some modelers have used Eq. (4)[4,5,6,7], whereas others have used Eq. (5)[8,9], as discussed by Brill[10].

A "linear model," by definition, has the form of Eq. (4) or (5) and models one spectral function

such as reflectance. More ambitiously, one may seek to model interactions involving the eye, a range of light sources *and* the population of reflectances, with the linear model as a starting point[1,4-6,9]. The goal of the larger model, almost by definition, is to predict a range of results with the fewest independent features such as basis functions.

Problem Statement: We seek to answer questions such as these:

1. Suppose that principal components analysis gives a mean vector and Q basis vectors. Is there a way to avoid the adding and subtracting of the mean vector and make a unity operator as in Eq. (2)?

2. When is the mean vector redundant with the Q basis vectors?

3. Principal component analyses of spectral reflectances have been published with[8,11] and without[12,13] the mean vector. Putting aside the model-building issue, how can a result with a mean vector be compared to another result without the mean?

The mean vector $|0\rangle$ bears no necessary relationship to the other vectors. We know that $\langle i|j\rangle = \delta_{ij}$, Eq. (1), but $\langle i|0\rangle$ can be zero or nonzero for each $\langle i|$. As stated, the mean vector is computed in an initial step, and then subtracted from each data vector before the calculation of the eigenvectors. The possibilities can be explored using fictitious examples. Each fictitious data vector has the form

$$|V_k\rangle=|0\rangle+c_{1k}|1\rangle+c_{2k}|2\rangle+...+c_{Qk}|Q\rangle \quad . \tag{6}$$

Once again, Q is the number of eigenvectors to be used in a working linear model, a small number such as 3. No coefficient multiplies the mean vector. Its contribution is the same for all k. In contriving the set of vectors, $\{|V_k\rangle\}$,

Case 1. We could arrange for $|0\rangle$ to be the constant zero, $|0\rangle = 0$. Making this substitution in Eq. (5) reduces it to Eq. (4). This is the desired result, but achieved in a narrow way.

Case 2. We could make $|0\rangle$ proportional to one of the basis vectors, say $|0\rangle = m_1|1\rangle$, where m_1 is a constant. More generally, the mean could be a linear combination of the other vectors,

$$|0\rangle = \sum_{j=1}^{Q} m_j |j\rangle \quad . \tag{7}$$

Case 3. Mean vector $|0\rangle$ could be a vector $|S\rangle$ that is orthogonal to the other vectors:

$$|0\rangle=|S\rangle, \langle S|j\rangle=0, j= 1, 2, ..., Q \, . \tag{8}$$

Case 4. Most generally, cases 2 and 3 can combine to give

$$|0\rangle = |S\rangle + \sum_{j=1}^{Q} m_j |j\rangle \quad , \tag{9}$$

where again $|S\rangle$ is orthogonal to the other vectors. (S = *senkrecht* = perpendicular. Uppercase $|S\rangle$ denotes this vector orthogonal to the basis functions, while lowercase $|s\rangle$ is the symbol for a **s**urface **s**pectral reflectance—any data vector.) Case 4 contains the simpler cases.

Case 2: Mean Vector Lies in PC Subspace

Case 2 is particularly interesting. Let Eq. (5) be written as

$$|s\rangle \approx |0\rangle + \sum_{j}^{Q} |j\rangle\langle j|\left(|s\rangle - |0\rangle\right) \quad . \tag{10}$$

Substituting for $|0\rangle$ from Eq. (7),

$$|s\rangle \approx \sum_{k=1}^{Q} m_k |k\rangle + \sum_{j=1}^{Q} |j\rangle\langle j| \left(|s\rangle - \sum_{k=1}^{Q} m_k |k\rangle \right) \quad . \tag{11}$$

Applying the orthonormality relationship of Eq. (1), $\langle j|k\rangle = \delta_{jk}$, then

$$|s\rangle \approx \sum_{k=1}^{Q} m_k |k\rangle + \sum_{j=1}^{Q} |j\rangle\langle j|s\rangle - \sum_{j=1}^{Q} m_j |j\rangle \quad . \tag{12}$$

The first and last terms on the right cancel:

$$|\sigma\rangle \approx \sum_{j=1}^{Q} |j\rangle\langle j|\sigma\rangle \quad . \tag{13}$$

Formally this is equivalent to Eq. (4), but it represents new knowledge. We see that if a linear model comes from a principal components method and therefore has the form of Eq. (5), but if the special condition of Eq. (7) is also satisfied, then we can get rid of the mean vector $|0\rangle$ in Eq. (10). And how do we get rid of it? Very simply, we erase it, throw it out.

In the most general case, to model vector $|s\rangle$, it is necessary to subtract $|0\rangle$, apply the unity operator to $(|s\rangle - |0\rangle)$, then add $|0\rangle$ back. In this special case, the mean vector is unchanged by the application of the unity operator, so that one may, if one wishes, omit the process of subtracting and adding.

Case 3: Mean Vector Orthogonal to PC Subspace

In the logic just developed, Case 3 is the opposite of Case 2. The application of the projection operator would cause $|0\rangle$ to vanish, so that Eq. (5) reduces to

$$|s\rangle \approx |0\rangle + \sum_{j}^{Q} |j\rangle\langle j|s\rangle \quad . \tag{14}$$

The remaining instance of $|0\rangle$ is the one that is not acted upon by the projection operator in Eq. (5). When the condition of Eq. (8) is met, an alternative path is to normalize $|0\rangle$, then make the normalized version one of the basis vectors. This converts Case 3 into Case 2. $|0\rangle$ is not added or subtracted as in Eq. (5), but the (normalized) mean vector is now wearing a wig and a dress and is disguised as a basis vector. One does not get something for nothing. Either the number of basis vectors is increased (from 3 to 4, for example), or else another basis vector must be thrown out.

Case 4: Unrestricted Mean Vector

Case 4, the general case, can be converted into Case 3 by finding a residual vector, r:

$$|r\rangle = |0\rangle - \mathbb{1}|0\rangle \quad . \tag{15}$$

Residual $|r\rangle$ is now orthogonal to the basis vectors $|1\rangle,|2\rangle,...|Q\rangle$ and can be substituted for $|0\rangle$ in Eq. (5), since by the logic of Case 2, the components $\mathbb{1}|0\rangle$ can be dropped. By the logic of Case 3, we could normalize $|r\rangle$ and make it one of the basis vectors, but there is another possibility, that $|r\rangle$ may be small enough to neglect.

To cast the projection operator in Eq. (15) in matrix form, if there are Q basis vectors, one may

write Eq. (2) as

$$\mathbb{1} = \begin{bmatrix} |1\rangle & |2\rangle \ldots & |Q\rangle \end{bmatrix} \begin{bmatrix} \langle 1| \\ \langle 2| \\ \vdots \\ \langle Q| \end{bmatrix} \quad . \tag{16}$$

Recall that $|j\rangle$ is a column vector, and $\langle j|$ is its transpose, a row vector.

We Rediscover Parseval's Theorem

How would one know if $|r\rangle$ is small? The approach is the same that applies to any orthogonal function expansion. Since $|r\rangle$ is a contribution to mean reflectance $|0\rangle$ that is orthogonal to the basis functions in the unity operator, the approximation looks like Eq. (14):

$$|s\rangle \approx |r\rangle + \sum_{j}^{Q} |j\rangle\langle j|s\rangle \quad . \tag{17}$$

To find the sum-squared value on both sides,

$$\langle s|s\rangle \approx \left(\langle r| + \sum_{i=1}^{Q} \langle i|s\rangle\langle i| \right) \left(|r\rangle + \sum_{j=1}^{Q} |j\rangle\langle j|s\rangle \right) \quad . \tag{18}$$

Multiplying Q+1 terms by Q+1 terms on the right gives $(Q+1)^2$ terms, but the orthogonality relationships save the day, reducing the terms to Q+1:

$$\langle s|s\rangle \approx \langle r|r\rangle + \sum_{j=1}^{Q} \langle j|s\rangle^2 \quad . \tag{19}$$

The Q terms added to $\langle r|r\rangle$ are the squared coefficients in the series expansion of $|s\rangle$. If the sum were not truncated at j=Q, but continued to P terms, the equality would be exact. (The limit on i must be increased before Eq. (15).) This equality is called Parseval's theorem. In textbooks on Fourier Series, the theorem is proved for an infinite sum of sine and cosine terms. The key step is the application of orthonormality between Eq. (18) and Eq. (19), so the theorem need not involve trigonometric functions. An infinite sum is not needed with a finite-dimensional space. In Eq. (19), $\langle s|s\rangle$ is the squared length of the reflectance vector, and each term on the right is the squared length of one orthogonal component.

Electrical engineers are traditionally taught a version of Parseval's theorem which says "The power in the waveform is the sum of the power in the harmonics." A mathematician may wince at this narrow statement, but to us who would be color engineers, it is a reminder that Parseval's theorem is an everyday practical matter. It is Pythagoras's ancient theorem about the square on the hypotenuse, extended to many-dimensional space. When curve-fitting results are assessed by the percentage of variance explained, this can be considered an indirect reference to Parseval's theorem.

Since the terms on the right in Eq. (19) are all ≥ 0, and adding terms would lead to equality, the equation can be written as an inequality,

$$\langle s|s\rangle \geq \langle r|r\rangle + \sum_{j=1}^{Q} \langle j|s\rangle^2 \quad . \tag{20}$$

The measure of whether $|r\rangle$ is negligible then is the size of $\langle r|r\rangle/\langle s|s\rangle$. This ratio could be

multiplied by 100% and called "percent of total squared length explained by $|r\rangle$." If $\langle s|s\rangle$ and the Q values $\langle i|s\rangle$ are known, then Eq. (20) sets a bound on $\langle r|r\rangle$ without necessarily calculating $|r\rangle$. Notice that functions $\langle i|$ are normalized, but $|r\rangle$, per Eq. (15), is not.

Ideally, one would like $\langle r|r\rangle$ to be negligible with respect to $\langle s_k|s_k\rangle$ for all known surfaces $|s_k\rangle$. A quick test is to ask if $|r\rangle$ is small with respect to the mean.

Nontrivial Example: Vrhel's Reflectance Data

Vrhel, Gershon and Iwan measured reflectances of 64 Munsell chips, 120 paint chips, and 170 miscellaneous items[8]. In the article, a mean vector and 7 principal components vectors are tabulated over the domain of 400 nm to 700 nm, at 10 nm intervals, based on all 354 samples. Via ftp, the PC vectors are available, along with all the raw data[8]. As supplied, the basis vectors are not normalized; they are orthogonal, so it is a simple matter to normalize each principal component:

$$|j\rangle \leftarrow |j\rangle/\langle j|j\rangle^{1/2} \quad . \tag{21}$$

It works best not to normalize the mean vector $|0\rangle$, for which $\langle 0|0\rangle = 2.5573$. Applying Eq. (20) to the case of the mean vector, the sequence of values $\langle j|0\rangle^2$ is [2.5307, 0.0136, 0.0068, 0.0045, 0.0003, 0.0001, 0.0005]. We can see immediately that $2.5307 \approx 2.5573$, meaning that if the mean vector is expanded in the basis of the other functions, the first term in the series gives a good fit, accounting for 98.961% of the squared length in the mean vector. A 3-term series accounts for 99.759%. (All 7 published vectors account for 99.970%.) Taking the residual vector $|r\rangle$ as the component of the mean not in the space of the first 3 terms, Eq. (15) and (16), leads to $\langle r|r\rangle = 0.0062$. Thus $\langle r|r\rangle$ is 0.2412% of $\langle 0|0\rangle$. Vrhel's results qualify for Case 2, defined by Eq. (7). That is, the mean vector is well fit by three or fewer of the principal components, and therefore

reflectances $|s\rangle$ are fit by a linear model in which the mean vector is absent, Eq. (13).

Moment of Reflection. The reader may feel that we have done quite a lot of algebraic thrashing around in order to achieve a baffling result, the principle that in certain cases Eq. (5) may be simplified by deleting $|0\rangle$ wherever it appears, even though $|0\rangle$ is not negligibly small. Why prove a crazy thing like that? The answer is that the stakes are rather high. On the one hand, the logic of principal components analysis says that we should subtract out the mean vector before computing the covariance matrix, leading to Eq. (5). On the other hand, we would like to have, as a tool for repeated use, a linear model with the simplicity of Eq. (4). In the case of Vrhel's large data set, the mean and principal components fall into Case 4 with $|r\rangle$ small, which we can treat as Case 2, a powerful simplification. With other data, a lesser simplification may apply.

Failure to convert a mean-centered PCA to a basis-function expansion can result in difficulties when the PCA is used within a larger model. Some application algorithms, such as linear models that approximate illuminant change in an image, require spectra to be approximated by a small number of basis spectra (e. g., three), each with a coefficient. In such applications, a redundant mean spectrum can waste a valuable degree of freedom. It might seem that the mean comes with a coefficient, gratis, namely "1", but that is not always true. Consider the PCA of daylight[14,15], in which the mean spectrum must be rescaled to fit each lighting situation. The scaling factor on the mean vector uses one degree of freedom, just like a coefficient of a basis vector.

Further Analysis

Our goal has not been to derive a single formula, but to work through some issues, raising the reader's awareness, and our own. In this context, we saw that if $|r\rangle$ is small, then the mean vector $|0\rangle$ can be dropped from Eq. (5) and Eq. (10). Without stating a precise criterion, we have shown in one example that $|r\rangle$ may indeed be small.

An open question is, suppose that $|r\rangle$ is not so clearly tiny; is it more significant than $|3\rangle$? More significant than $|4\rangle$? Principal component functions are always ranked according to their utility in explaining the original data vectors. To treat $|r\rangle$ as an additional basis vector, Case 4 above, one would like to know where it falls into the sequence of principal components. Let us add detail to Eq. (20), applying it to each surface $|s_i\rangle$ in the original principal-component analysis:

$$\langle s_i | s_i \rangle \geq \sum_{j=1}^{Q} \langle s_i | j \rangle^2 + \langle r(Q) | r(Q) \rangle \quad . \tag{22}$$

We wish to make a linear model of exactly Q basis vectors. Then $|r(Q)\rangle$ is found by Eq. (15), with projection operator $\mathbb{1}$ based on the first Q basis functions. Mean-residual $|r\rangle$ is written as $|r(Q)\rangle$ in order to emphasize a key idea. As in any basis function expansion, $|j\rangle$ and the associated coefficient $\langle s_i|j\rangle$ are independent of Q, the number of terms kept in the approximation, Eq. (17). In contrast, $|r\rangle$ depends on Q.

Eq. (22) holds for each of the original M data vectors $|s_i\rangle$, $i = 1, 2, \ldots M$. Adding all M instances gives a single inequality with contributions on the right side due to each of the basis vectors, and to the residual:

$$\sum_{i=1}^{M} \langle s_i | s_i \rangle \geq u_1 + u_2 + \ldots + u_Q + v \quad , \tag{23}$$

where

$$u_j = \sum_{i=1}^{M} \langle s_i | j \rangle^2 \tag{24}$$

is the sum of square contributions from the data in direction $|j\rangle$, and

$$v = \sum_{i=1}^{M} \langle r(Q) | r(Q) \rangle = M \langle r(Q) | r(Q) \rangle \tag{25}$$

is the sum of squared contributions of the residual.

The residual should displace the least significant basis function, $|Q\rangle$, only if its contribution to the total sum of squares is greater than that of $|Q\rangle$. That is, $|r(Q)\rangle$ should displace $|Q\rangle$ if

$$M \langle r(Q) | r(Q) \rangle > \sum_{i=1}^{M} \langle s_i | Q \rangle^2 \quad . \tag{26}$$

The inequality in Eq. (26) does not relate to that in Eq. (23), which is always true. Eq. (26) tests which is the larger contribution, u_Q or $v(Q)$. If the data vectors $|s_i\rangle$ are collected into the columns of matrix $\mathbf{X}_{N\times M}$, then $\mathbf{C} = \mathbf{X}'|Q\rangle$ is a column vector of the coefficients $\langle s_i|Q\rangle$ and $\mathbf{C}'\mathbf{C}$ is the indicated sum of coefficients squared. We analyzed Vrhel's set of 354 data vectors, recorded at 2-nm intervals[8] over the domain 390 to 730 nm, to find the mean vector and principal components.

Then, stepping integer Q from 1 to 10, we computed $|r(Q)\rangle$ and then the quantities on the left and right of Eq. (26). In Table I, these quantities are compared, and additional columns show the eigenvalues of the original covariance matrix and also $\sum\langle s_{\text{reduced}}|Q\rangle^2$. This last quantity is the sum of squared coefficients in the Qth column of a similar coefficient matrix **C**, *if* the coefficients are found for the "reduced" data set, $\langle s|-\langle 0|$.

In Table I, we see that inequality (26) is false for all 10 values of index Q. This means that the residual should not be used for any linear model requiring 1 or 2 or 3 up to 10 basis vectors.

Table I. Analysis of Vrhel's data for the significance of the mean-residual.

index Q	M⟨r|r⟩	$\sum\langle s\|Q\rangle^2$	eigenvalue	$\sum\langle s_{\text{reduced}}\|Q\rangle^2$
1	80.389	7785.841	2448.123	2448.123
2	58.607	697.121	675.338	675.338
3	39.813	198.265	179.471	179.471
4	4.226	74.000	38.412	38.412
5	4.124	22.697	22.596	22.596
6	3.405	10.280	9.561	9.561
7	0.770	8.747	6.112	6.112
8	0.770	4.511	4.510	4.510
9	0.346	2.185	1.760	1.760
10	0.338	1.462	1.455	1.455

While the numbers are of no lasting interest, this table illustrates the concept of linear models and the specific ideas concerning the mean vector. Because the last column is $M-1$ times the variance

of the data in the Qth principal direction $|Q\rangle$, the equality of the last two columns bears out the well-known fact[9] that the Qth eigenvalue is proportional to the total variance in the $|Q\rangle$ direction. The last column arises from modeling the exact data, with the mean subtracted, from which the basis functions were derived. By contrast, the column $\sum\langle s|Q\rangle^2$ arises when we use the same basis functions to model something different: the original data with the mean not subtracted. These numerical results are an exemplar for what we hope will happen when the same model is applied to new data sets. We hope that, although the explanatory value of each vector, expressed by $\sum\langle s|Q\rangle^2$, will be altered, the general pattern will remain. That is, the first vector, $|1\rangle$, will be most explanatory, and the first few vectors together will explain a large fraction of the variation in the new data.

Table I concerns a case—Vrhel's data—that is a close approximation to our hypothetical Case 2, in which the mean is a linear combination of the Q eigenvectors. If we imagine a data set conforming to Case 3, where the mean vector is orthogonal to all of the Q eigenvectors, the appearance of the table would differ. The mean as a component of each data vector would be invisible to the calculation of $\langle s|Q\rangle$, so the numbers $\sum\langle s|Q\rangle^2$ would equal the eigenvalues. Three columns would be the same. At the same time, the mean-residual $|r\rangle$ would equal the mean. The mean cannot be small for all-positive data such as reflectances, so the numbers in the first column would be larger and not decreasing with increasing Q. Inequality (26) would be satisfied for some or all values of $|Q\rangle$, mandating that a normalized $|r\rangle$ become one of the basis functions.

Conclusion

This article has concerned the case that one wishes to construct a linear model based on principal components analysis of data vectors such as spectral reflectances. The most striking conclusion,

embodied in Eq. (13) and its context, is that a model based on Q eigenvectors can be simplified if the mean vector of the original data happens to be a linear combination of the Q eigenvectors. When the Q eigenvectors fit the mean vector closely but not exactly, inequality (26) offers a test, whether the fit is close enough so that the simplification can be used. No originality is claimed for these results. Others must have made similar observations. Our goal has been to develop some ideas in a tutorial way, to facilitate the use of principal components in color science.

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