Mathematical derivation for Vora-Value based filter design method: Gradient and Hessian

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Abstract: In this paper, we present the detailed mathematical derivation of the gradient and Hessian matrix for the Vora-Value based colorimetric filter optimization. We make a full recapitulation of the steps involved in differentiating the objective function and reveal the positive-definite Hessian matrix when a positive regularizer is applied. This paper serves as a supplementary material for our paper in the colorimetric filter design theory.

Keywords: Optimization method; Gradient descent; Newton method; Vora-Value

1. Preliminary

Let \( Q = [r, g, b] \) and \( X = [x, y, z] \) denote respectively the spectral sensitivities of the camera and the CIE XYZ color matching functions (CMFs) of the human visual sensors. The columns of matrices \( Q \) and \( X \) represent the spectral sensitivity for each sensor channel and the rows represent the sensor responses at a sampled wavelength. Both matrices are in the size of \( n \times 3 \), where \( n \) is the number of sampling wavelengths across the visible spectrum.

1.1. Notation

We will use the following notation for the gradient and Hessian matrix (with respect to the \( n \)-dimensional filter vector \( f = [f_1, f_2, \ldots, f_n]^T \)):

\[
\nabla \nu(f) = \begin{bmatrix} \frac{\partial \nu}{\partial f_1} \\ \vdots \\ \frac{\partial \nu}{\partial f_n} \end{bmatrix}
\]

and

\[
H = \nabla^2 \nu(f) = \begin{bmatrix} \frac{\partial^2 \nu}{\partial f_1^2} & \frac{\partial^2 \nu}{\partial f_1 \partial f_2} & \cdots & \frac{\partial^2 \nu}{\partial f_1 \partial f_n} \\ \frac{\partial^2 \nu}{\partial f_2 \partial f_1} & \frac{\partial^2 \nu}{\partial f_2^2} & \cdots & \frac{\partial^2 \nu}{\partial f_2 \partial f_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 \nu}{\partial f_n \partial f_1} & \frac{\partial^2 \nu}{\partial f_n \partial f_2} & \cdots & \frac{\partial^2 \nu}{\partial f_n^2} \end{bmatrix}
\]

or equivalently, using the indices, we can respectively express as \((\nabla \nu)_i = \frac{\partial \nu}{\partial f_i}\) and \(H_{ij} = \frac{\partial^2 \nu}{\partial f_i \partial f_j}\) [1]. From the definitions, we know that \( \nabla \nu \) and \( \nabla^2 \nu \) are respectively in the size of \( n \times 1 \) and \( n \times n \).

1.2. Vora-Value

Given a camera sensor set \( Q \) and the trichromatic human visual sensors \( X \), the Vora-Value is defined [2] as

\[
\nu(Q, X) = \frac{1}{3} tr(Q(Q^TQ)^{-1}Q^TX(X^TX)^{-1}X^T)
\]
where the superscripts $^T$ and $^{-1}$ denote respectively the matrix transpose and inverse and $tr()$ returns the sum of the elements along the diagonal of a matrix. The Vora-Value is often used to measure how similarly a camera samples the spectral signals compared to the human visual system. It returns a number in the range $[0,1]$ where 1 means the camera is fully colorimetric such that RGBs are precisely a linear transform from XYZ tristimulus values. A higher Vora-Value indicates a better fit between two sensor systems.

1.3. Projector Matrix

The projector of a matrix - such as $Q$ - is defined as

$$P\{Q\} = Q(Q^TQ)^{-1}Q^T.$$ (3)

When we return to Eq. (2), it can also be written in a more compact representation as

$$\nu(Q,X) = 1/3 tr(P\{Q\}P\{X\}).$$ (4)

where $P\{Q\}$ and $P\{X\}$ denote the projection matrices respectively of the camera spectral sensitivities $Q$ and the human visual responses $X$.

1.4. Orthonormal Basis

In an $n$-dimensional vector space, $n$ linearly independent vectors forms a set. We call such a set as basis set. Every vector in the $n$-dimensional vector space can be expressed as a linear combination of the basis vectors. There are infinite bases for a vector space and, by definition, they are all linear transform apart.

Let $V = [v_1, v_2, v_3]$ denote a special linear combination of $X = [x, y, z]$ as

$$V = XT$$ (5)

where $T$ is the (full rank) linear mapping matrix which makes $V$ orthonormal. An orthonormal matrix has columns that are unit vectors and also perpendicular to each other. Mathematically, we write $V^TV = I_3$ ($I_3$ is the $3 \times 3$ identity matrix). The orthonormal matrix $V$ can be obtained by many methods, e.g. the Gram-Schmidt process [3].

By simple substitution into the matrix projector in Eq. (3), we can express projector matrices in a simpler algebraic form:

$$P\{X\} = P\{V\} = VV^T$$ (6)

and then substituting into Eq. (2), we can simplify the Vora-Value as

$$\nu(Q,X) = \nu(Q,V) = 1/3 tr(Q(Q^TQ)^{-1}Q^TVV^T).$$ (7)

1.5. Filter-modified Vora-Value

Previously, we proposed to design a color filter which, when placed in front of a camera, can make the new effective camera more colorimetric [4]. When a color filter is placed in front of a camera, it alters the spectral sensitivities. The effect of placing a color filter to a camera can be modeled as the multiplication of the filter spectral transmittance to the camera spectral sensitivities. Given an $n$-dimensional filter vector (with $f_i > 0$) and camera spectral sensitivity matrix $Q$, the new effective sensitivity responses after filtering can be represented as $\text{diag}(f)Q$. To ease the notation, we use $F = \text{diag}(f)$ and rewrite as $FQ$. 

Thus the filter-modified Vora-Value for the effective 'filter+camera' system (using the orthonormal basis of the XYZ CMFs) can be written as

$$\nu(F_Q, X) = \frac{1}{3} tr(F_Q(Q^T F^2 Q)^{-1} Q^T F V V^T).$$

(8)

Or equivalently, in the simpler representation (using projector matrices), we write $$\nu(F_Q, X) = \frac{1}{3} trace(P\{F_Q\} P\{X\}).$$

2. Derivation of Gradient

In this section, we will derive the gradient, in terms of the filter vector, of the filter-modified Vora-Value as given in Eq. (8).

**Theorem 1.** \( \nabla \nu(f) = \frac{\partial \nu}{\partial F} = \frac{2}{3} ed \text{dia}g \left( F^{-1} P\{F_Q\} P\{X\} \{I - P\{F_Q\}\} \right) \)

**Proof.** The following rules of matrix calculus are used to obtain the required differentials:

$$d \text{tr}(U) = \text{tr}(dU)$$
$$d(UV) = U dV + dU V$$
$$d(AU) = A dU$$
$$dU^{-1} = -U^{-1}(dU)U^{-1}$$

(9)

Using the above rules, we have

$$d\nu(F) = \frac{1}{3} tr \left( dF Q(Q^T F^2 Q)^{-1} Q^T F V V^T - 2FQ(Q^T F^2 Q)^{-1} Q^T F dF Q(Q^T F^2 Q)^{-1} Q^T F V V^T + FQ(Q^T F^2 Q)^{-1} Q^T dF V V^T \right).$$

(10)

Using the acyclic property of trace that \( \text{tr}(ABC) = \text{tr}(BCA) = \text{tr}(CAB) \), we can move the \( dF \) in each of the term to the end of the formulation. We also use the projector representation of \( P\{X\} = V V^T \) to make it more compact as

$$d\nu(F) = \frac{1}{3} tr \left( Q(Q^T F^2 Q)^{-1} Q^T F P\{X\} dF - 2Q(Q^T F^2 Q)^{-1} Q^T F P\{X\} FQ(Q^T F^2 Q)^{-1} Q^T F dF + P\{X\} FQ(Q^T F^2 Q)^{-1} Q^T dF \right).$$

(11)

Using the diagonal property of \( F \) is defined, we can make the derivative as

$$\frac{\partial \nu(F)}{\partial F_{ii}} = \frac{1}{3} \left[ Q(Q^T F^2 Q)^{-1} Q^T F P\{X\} - 2Q(Q^T F^2 Q)^{-1} Q^T F P\{X\} FQ(Q^T F^2 Q)^{-1} Q^T F + P\{X\} FQ(Q^T F^2 Q)^{-1} Q^T \right]_{ii}$$

(12)
We use $F^{-1}P\{FQ\} = Q(Q^TF^2Q)^{-1}Q^TF$ to ease the notation (the diagonality of $F$ guarantees it to be invertible). Our gradient function can be expressed as

$$\frac{\partial \nu(F)}{\partial F_{ii}} = \frac{1}{3} \left[ F^{-1}P\{FQ\}P\{X\} - 2F^{-1}P\{FQ\}P\{X\}P\{FQ\} + P\{X\}P\{FQ\}F^{-1} \right]_{ii}$$

(13)

Given $F^{-1}P\{FQ\}P\{X\}$ is symmetric, we have

$$\frac{\partial \nu(F)}{\partial F_{ii}} = \frac{2}{3} \left[ F^{-1}P\{FQ\}P\{X\} - F^{-1}P\{FQ\}P\{X\}P\{FQ\} \right]_{ii}$$

(14)

This equation can be further merged into

$$\frac{\partial \nu(F)}{\partial F_{ii}} = \frac{2}{3} \left[ F^{-1}P\{FQ\}P\{X\}(I - P\{FQ\}) \right]_{ii}$$

(15)

where $I$ is the identity matrix.

Now, let us rewrite the derivative in terms of the underlying filter vector $f$. First, remember that $F = \text{diag}(f)$. Let us denote the inverse operator - the one that extracts the diagonal from a square matrix and places the result in a vector - as $\text{ediag}$ ('e' signifies to ‘extract’ the diagonal elements). Clearly, $\text{ediag} \left( \text{diag}(f) \right) = f$. Here, $\text{diag}()$ is a forward operation turning a vector into a diagonal matrix and $\text{ediag}$ is the companion reverse operator extracting the diagonal.

Now we can derive the gradient, in terms of the underlying filter vector, as

$$\nabla \nu(f) = \frac{\partial \nu(F)}{\partial f} = \frac{2}{3} \text{ediag} \left( F^{-1}P\{FQ\}P\{X\}(I - P\{FQ\}) \right)$$

(16)

where the gradient with respect to the filter vector, $\nabla \nu(f)$, is a $n \times 1$ vector.

It is evident that the gradient has a very interesting structure: it is the diagonal of the product of three projection matrices multiplied by the inverse of the filter (at hand). We will come back to this interesting feature later.

2.1. Smoothness Constrained Filter

When the filter is composed by a linear combination of a set of basis functions, $f = Bc$ where columns of $B$ are basis vectors and $c$ denotes the coefficients [5]. By using the chain rule, we can calculate the gradient with respect to the coefficient vector $c$ as:

$$\nabla \nu(c) = B^t \frac{\partial \nu(F)}{\partial f}$$

(17)

or, equivalently in its explicit form as

$$\nabla \nu(c) = \frac{2}{3} B^t \text{ediag} \left( F^{-1}P\{FQ\}P\{X\}(I - P\{FQ\}) \right)$$

(18)

2.2. Filter Design with Regularization

In Eq. (19), we reformulate the filter design optimization that we aim to minimize (instead of to maximize as for the Vora-Value optimization):

$$\mu(F) = -\text{tr}(P\{FQ\}P\{X\}) + \alpha \| F \|^2_2.$$

(19)
In contrast to the Vora-Value optimization, we reverse to the negative and cancel the fractional scalar in the equation. Here we use the symbol $\mu$ to denote the new objective function with a regularization term. The penalty term that we introduce here is the squared norm of the filter where $\alpha > 0$.

Clearly, we have the following relation of the gradient: $\nabla \mu(f) = -3\nabla \nu(f) + 2\alpha f$. Therefore, the gradient of the regularized optimization is written as

$$\nabla \mu(f) = -2\text{diag} \left( F^{-1}P\{FQ\} P\{X\}(I - P\{FQ\}) \right) + 2\alpha f. \quad (20)$$

3. Derivation of Hessian Matrix

Here we present how we derive the second derivative - the Hessian matrix - of our objective function given in Eq. (19). The Hessian matrix makes a further derivative of Eq. (20). As the second derivative will have many terms in the equation, to ease the notation, we use $A$, $B$ and $C$ to respectively denote $P\{X\}$, $P\{FQ\}$, $F^{-1}$ hereafter.

Now we differentiate for the second derivative using the matrix calculus laws in Eq. (9):

$$d^2 \mu = tr(-2CB dF CBA dF + 2CB dF CBAB dF$$
$$+ CBC dF A dF - CBC dF AB dF$$
$$- CBA dF CB dF + 2CBAB dF CB dF$$
$$- CBABC dF dF) + 2\alpha dF dF \quad (21)$$

After further merging between two terms in each line, we obtain

$$d^2 \mu = tr(-2CB dF CBA (I - B) dF$$
$$+ CBC dF A (I - B) dF$$
$$- CBA (I - 2B) dF CB dF$$
$$- CBABC dF dF) + 2\alpha dF dF \quad (22)$$

where $I$ denotes the $31 \times 31$ identity matrix.

Given $f = \text{diag}(F)$ and any two square matrices $M$ and $N$, we have $tr(M^T dF N dF) = \sum_{i,j} M_{ij} N_{ij} df_i df_j$ where elements having the same indices in two matrices are multiplied. Using this property into Eq. (22) and the symmetric property of matrices $A, B, C$ (as projector matrices and the diagonal filter matrix $F$ are symmetric), we can derive the Hessian matrix as

$$H = -2 \left( BC \right) \circ \left( (I - B)ABC \right) + \left( CBC \right) \circ \left( (I - B)A \right)$$
$$+ \left( (I - 2B)ABC \right) \circ \left( BC \right) - \left( CBABC \right) \circ I + 2\alpha I \quad (23)$$

where $\circ$ denotes the Hadamard product (or elementwise product) of two matrices, i.e. $(M \circ N)_{i,j} = M_{i,j}N_{i,j}$. The explicit expansion of the equation over projector matrices are written as
\[
H = -2(P_{FQ}F^{-1}) \circ ((I - P_{FQ})P_{X}P_{FQ}F^{-1}) \\
+ (F^{-1}P_{FQ}F^{-1}) \circ (P_{X}P_{FQ}F^{-1}) \\
+ (I - 2P_{FQ})P_{X}P_{FQ}F^{-1} \circ (P_{FQ}F^{-1}) \\
+ (F^{-1}P_{FQ}P_{X}P_{FQ}F^{-1}) \circ (P_{FQ}F^{-1}) \\
+ 2\alpha I
\] (24)

where the last term relates to the regularization term.

4. Positive Definiteness of Hessian Matrix

The gradient of the Vora-Value based objective function (when we discount the regularizer) has an interesting structure as given in Eq. (16). It is the product of three projector matrices and the inverse of the filter matrix. We find that the filter vector, \( f \), and the gradient, \( \nabla \nu(f) \), are perpendicular to each other. That is, when we multiply \( f^T \) to it, we have

\[
f^T \nabla \nu(f) = f^T \text{ediag}((I - P_{FQ})P_{V}P_{FQ}F^{-1}) = 0.
\]

Therefore, given this property, we have

\[
f^T \nabla \mu(f) = f^T (-3 \nabla \nu(f) + 2\alpha f) = 2\alpha f^T f
\] (25)

Now, if we make the derivative to the both sides of Eq. (25) with respect to \( f \), we obtain

\[
\nabla \mu + (\nabla^2 \mu) f = 4\alpha f.
\] (26)

If we multiply \( f^T \) to this equation, we have

\[
f^T \nabla \mu + f^T (\nabla^2 \mu) f = 4\alpha f^T f.
\]

From Eq. (25), we know

\[
f^T \nabla \mu(f) = 2\alpha f^T f.
\]

Hence, we get

\[
f^T (\nabla^2 \mu) f = 2\alpha f^T f > 0, \quad \text{if} \quad \alpha > 0
\] (27)

which guarantees the Hessian to be positive definite under a positive regularizer \( \alpha \) (and also a physically plausible filter is a non-zero vector, \( f > 0 \)). The positive-definite property ensures the Hessian matrix to be invertible and thus we can use the Newton’s method - which involves the inverse of the Hessian matrix [6] - for the Vora-Value based filter optimization.

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