Question: How did Jozef Cohen derive the formula $\mathbf{R} = A(A'A)^{-1}A'$?

Cohen's Derivation of Matrix **R**

Consider a set of K linearly independent column vectors q_i of length M. In color work, one might have $K = 3$ and $M = 471$, or $M = 31$, for example. The vectors could be color matching functions or something else. It is assumed in any event that $K < M$. The vectors q_i are the columns of matrix $A_{M\times K}$. If $K = 3$,

$$A = \begin{bmatrix} q_1 & q_2 & q_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ \vdots & \vdots & \vdots \end{bmatrix} . \tag{1}$$

Then let N be an arbitrary vector of length M. In color work, it might represent the spectral distribution of a light. It is then desired to find a vector N^* which is a linear combination of the columns of A, and a least-squares best fit to N. [In other words, if the columns of A are color matching functions, N^* is the fundamental metamer. The asterisk has nothing to do with complex conjugate or Hermitian. Matrix transpose will be indicated below by the prime symbol, '.]

For illustration, let K=3, but the derivation will apply for any K<M. Then the columns of A are linearly combined according to the coefficients U:

$$U = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} . \tag{2}$$

That is,

$$N^* = AU . \tag{3}$$

Eq. (3) expresses the idea that N^* is a linear combination of the vectors q_i . Then the least-squares condition must be applied. Expressing Eq. (3) in more detail,

$$\begin{bmatrix} a_{11}u_1 + a_{12}u_2 + a_{13}u_3 \\ a_{21}u_1 + a_{22}u_2 + a_{23}u_3 \\ a_{31}u_1 + a_{32}u_2 + a_{33}u_3 \\ a_{41}u_1 + a_{42}u_2 + a_{43}u_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} n^*_1 \\ n^*_2 \\ n^*_3 \\ n^*_4 \\ \vdots \end{bmatrix} . \tag{4}$$

To minimize the vector distance from N to N^*, $|N-AU|$ must be minimized, which is to say one must minimize the following sum of squares, SS:

$$\text{SS} = \quad (n_1 - [a_{11}u_1 + a_{12}u_2 + a_{13}u_3])^2 +$$

$$(n_1-[a_{21}u_1 + a_{22}u_2 + a_{23}u_3])^2 +$$
$$(n_1-[a_{31}u_1 + a_{32}u_2 + a_{33}u_3])^2 +$$
$$(n_1-[a_{41}u_1 + a_{42}u_2 + a_{43}u_3])^2 + ... \quad . \tag{5}$$

Now define $D = N - AU$, so that $d_j = n_j - [a_{j1}u_1 + a_{j2}u_2 + a_{j3}u_3]$.

With this substitution,

$$SS = d_1^2 + d_2^2 + d_3^2 + d_4^2 + ... \quad . \tag{6}$$

Taking the partial derivatives with respect to u_1, u_2, and u_3 and setting them equal to zero gives

$$\partial SS/\partial u_1 = -2a_{11}d_1 - 2a_{21}d_2 - 2a_{31}d_3 - ... = 0$$
$$\partial SS/\partial u_2 = -2a_{12}d_1 - 2a_{22}d_2 - 2a_{32}d_3 - ... = 0 \tag{7}$$
$$\partial SS/\partial u_1 = -2a_{13}d_1 - 2a_{23}d_2 - 2a_{33}d_3 - ... = 0 \quad .$$

Eq. (7) amounts to a 3-element vector set equal to zero. Dividing through by the factor of −2 and then expressing the result as a matrix product,

$$A'D = 0 \quad . \tag{8}$$

However, $D = N-AU$. Thus

$$A'(N-AU) = 0 \tag{9}$$

$$A'N - A'AU = 0 \tag{10}$$

$$A'AU = A'N \tag{11}$$

$$U = (A'A)^{-1}A'N \quad . \tag{12}$$

We sought an expression for N^*, which equals AU. Therefore,

$$N^* = AU = A(A'A)^{-1}A'N \quad . \tag{13}$$

In Eq. (13), we see that $A(A'A)^{-1}A'$ is the orthogonal projector projecting N into the three-space of the color mixture functions, or other column vectors in A. In short,

$$\mathbf{R} = A(A'A)^{-1}A' \quad . \tag{14}$$

Eq. (14) is the desired result.

The proof above is taken from Jozef B. Cohen and William E. Kappauf, "Metameric color stimuli, fundamental metamers, and Wyszecki's metameric blacks," *Am. J. Psych.* **95**(4):537-564 (1982). I have taken some liberty with the wording, but the proof is Cohen's.
JAW