Finding the Nearest Orthonormal Matrix

In some appoaches to photogrammetric problems (perhaps inspired by projective geometry), an estimate M of an orthonormal matrix R representing rotation is recovered. It is then desired to find the "nearest" orthonormal matrix. While this two step approach — first finding a "best fit" matrix without enforcing orthonormality, and then finding the nearest orthonormal matrix — is not to be recommended, it may be of interest to find a solution to this problem nevertheless.

So, given a matrix M, find the matrix R that minimizes $\|M - R\|_F^2$, subject to $R^T R = I$, where the norm chosen is the Frobenius norm, i.e. the sum of squares of elements of the matrix, or

$$\|X\|_F^2 = \text{Trace}(X^T X)$$

We can deal with the orthogonality contraint by introducing a symmetric Lagrangian multiplier matrix Λ and looking for stationary values of

$$e(R, \Lambda) = \text{Trace}\big((M - R)^T (M - R)\big) + \text{Trace}\big(\Lambda(R^T R - I)\big)$$

Now define the derivative of a scalar w.r.t. to a matrix to be the matrix of derivatives of the scalar w.r.t. to each of the component of the matrix. Then it is easy to derive the following useful identities [Horn 1986]

$$\frac{d}{dX}\text{Trace}(X) = I \quad \text{and} \quad \frac{d}{dX}\text{Trace}(X^T X) = 2X$$

$$\frac{d}{dA}\text{Trace}(AB) = B^T \quad \text{and} \quad \frac{d}{dB}\text{Trace}(AB) = A^T$$

$$\frac{d}{dX}\text{Trace}(AXB) = A^T B^T \quad \text{and} \quad \frac{d}{dX}\text{Trace}(AX^T X) = X(A + A^T)$$

Differentiating $e(R, \Lambda)$ w.r.t. R and setting the result equal to zero yields

$$-2(M - R) + R(\Lambda + \Lambda^T) = 0$$

or, since $\Lambda^T = \Lambda$,

$$-(M - R) + R\Lambda = 0$$

solving for M we get

$$M = R(I + \Lambda)$$

which is a useful decomposition of M into the product of an orthonormal and a symmetric matrix [Horn *et al* 1988]. Now

$$M^T M = (I + \Lambda) R^T R (I + \Lambda) = (I + \Lambda)^2$$

Hence

$$(I + \Lambda) = (M^T M)^{1/2}$$

and so, finally,

$$R = M(I + \Lambda)^{-1} = M(M^T M)^{-1/2}$$

Note that $M^T M$ is symmetric, non-negative definitive and so will have non-negative real eigenvalues. The inverse of the square root of $M^T M$ can thus be computed using eigenvalue-eigenvector decomposition. The inverse of the square root of $M^T M$ has the same eigenvectors as $M^T M$, and eigenvalues that are the inverse of the square roots of the eigenvalues of $M^T M$, so we can write

$$(M^T M)^{-1/2} = \frac{1}{\sqrt{\lambda_1}}\mathbf{e}_1\mathbf{e}_1^T + \frac{1}{\sqrt{\lambda_2}}\mathbf{e}_2\mathbf{e}_2^T + \frac{1}{\sqrt{\lambda_3}}\mathbf{e}_3\mathbf{e}_3^T$$

where λ_i for $i = 1$, 2, and 3, are the eigenvalues and $\mathbf{e}_i$ for $i = 1$, 2, and 3, are the eigenvectors of $M^T M$. This construction of the inverse of the square root of $M^T M$ fails if one of the three eigenvalues is zero. It is possible however to pretend that that eigenvalue is equal to one and proceed anyway [Horn *et al* 1988].

It is easy to verify that R constructed as above is orthonormal, i.e. $R^T R = I$. However, there is no guarantee that $\det(R) = +1$. To represent a proper rotation, the orthonormal matrix R has to satisfy this condition as well. Otherwise it represents a reflection, not a rotation. There is no easy way to enforce this condition, and with poor measurements, the estimated "rotation matrix" M may very well lead to a least squares solution R such that $\det(R) = -1$.

The "two stage method" of first fitting a matrix without enforcing orthonormality, followed by finding an orthonormal matrix that is "nearest" to the fitted matrix, produces a result that is less accurate than that obtained by solving the least-squares problem directly. Further, in general least squares fitting problems are solved more easily, and without the possibility of obtaining an improper rotation, using a better notation for rotation, such as unit quaternions [Horn 1987].

References

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