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Testing Matrices for Definiteness and Application Examples That Spawn the Need

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Introduction

IN a recent Note,[1] Prussing correctly observed via counterexamples that the "principal minor test" can lead to erroneous conclusions when used as publicized by several textbooks.[2-4] The version under scrutiny here and in Ref. 1 had been advertised to be a necessary and sufficient test to determine whether a symmetric matrix ($A = A^T$) and/or an Hermetian matrix ($A = \bar{A}^T$, where the vinculum denotes the complex conjugate) is positive semidefinite (c.f., Ref. 48). In fact, the conventional wisdom on this crucial test is incorrect, even though it had been propagated by the above-mentioned text-books (similar textbook misrepresentations on this subject[5-9] were further identified in Ref. 10). Additional splendid counterexamples can be constructed using the results of Ref. 13. Since Swamy[10] first alerted the control and estimation community to this error in 1973, a whole new crop of analysts has now sprung up apparently to repeat this same error for which his correction was, perhaps, not spread widely enough.

The fourfold purpose of this Note is:

1) To enthusiastically endorse the corrections of Prussing[1] and Swamy,[10] even though they limited their attention/observations to the effect of testing matrices only for positive *semidefiniteness*.

2) To list additional textbooks that have unfortunately inherited and further propagated this same mistake (offered here as a cautious reminder of which expert opinions to be wary of on this subject).

3) To provide an indication of why this issue is so important in applications (an emphasis that appears to be lacking in Refs. 1 and 10).

4) To describe an easily understood and accessible numerical technique that can serve as the foundation for a computer-based test for positive definiteness/semidefiniteness (as is needed for realistically handling the higher-dimensioned matrices typically encountered in practical industrial applications). The test recommended here differs from the *corrected/augmented* "principal minor test" offered in Refs. 1 and 10 (which is typically applicable only to long-hand calculations for the relatively low-dimensional matrices considered in classroom examples with "nice" numbers).

While the corrected/augmented positive semidefiniteness test offered in Refs. 1 and 10 could also be used as the basis of a numerical test procedure to be implemented on the computer to handle higher-dimensional practical problems, it would require several determinant evaluations that are notoriously computationally unwieldy and probably numerically ill-conditioned. The alternative test offered here is apparently more computationally efficient and numerically well-behaved for this type of application.

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Distinguishing the Correct Version

Now that the first purpose of this Note is satisfied, the second purpose is completed by indicating that Ref. 14 (p. 552) and Ref. 15 (pp. 381–382) are, unfortunately, also in error along the same lines as warned against in Refs. 1 and 10. Especially insightful engineering treatments/justification of the correct version of this positive semidefinite test are found, for example, in statements following Eqs. 12.3 in Ref. 44 (pp. 482–483), in Ref. 47 (pp. 384–385), Ref. 11 (p. 307), Ref. 16 (pp. 267–270), Ref. 17 (p. 46), and Ref. 18 (pp. 73–74).

Application Utility

As aptly indicated in Refs. 19–24 with coverage of multitudinous practical navigation and aerospace applications of Kalman filtering (and its mathematical dual of the optimal feedback regulator control of a linear system having the property of minimizing an integral quadratic cost function over either a finite or infinite planning horizon), optimal linear filtering and optimal feedback regulation[25-27] both require the solution of similar Riccati differential equations. For the case of continuous-time linear filtering, the associated Riccati equation is of the form,

$$\dot{P} = F(t)P + PF^T(t) + G(t)Q(t)G^T(t) - PH^T(t)R^{-1}(t)H(t)P \qquad (1)$$

with symmetric positive definite initial condition

$$P(t_0) = P_0 \qquad (2)$$

For Eq. (1), the system matrix $F(t)$, the noise gain matrix $G(t)$, and the process noise covariance intensity matrix $Q(t)$ are defined further below as they occur in the linear system model of Eq. (4). To simplify the discussion, Eqs. (4) and (5) depict a system with time-invariant matrices. As needed in order to employ optimal Kalman filtering, the sensor measurements should be capable of being adequately characterized mathematically as

$$y(t) = H(t)x(t) + v(t) \qquad (3)$$

where $H(t)$ is the observation matrix and $v(t)$ the zero mean Gaussian white measurement noise. $R(t) = R^T(t)$, which is the covariance intensity level of the white measurement noise $v(t)$. To be useful in applications, the solution $P(t)$ of the above Riccati equation must be at least positive semidefinite.

As in Ref. 28 (pp. 39–41), consider the time-invariant linear system of the form,

$$\dot{x}(t) = Fx(t) + Gu(t) \qquad (4)$$

$$y(t) = Hx(t) \qquad (5)$$

where $u(t)$ is the zero mean Gaussian white process noise (Ref. 28 instead utilizes the equivalent, but more mathematically rigorous, Brownian motion representation of the process noise) and $Q=Q^T$ is the covariance intensity level (being a positive definite matrix) of the white process noise $u(t)$.

Reference 28 indicates that the second-order statistics for the above system can be represented in the time and frequency domains, respectively, by the following matrix concatenations:

$$R_{yy}(t,\tau)=He^{F(t-\tau)}PH^T \text{ for } t>\tau \tag{6a}$$

$$=HPe^{F^T(\tau-t)}H^T \text{ for } \tau\geq t \tag{6b}$$

and

$$S_{yy}(j\omega)=H(j\omega I-F)^{-1}GQG^T(-j\omega I-F^T)^{-1}H^T \tag{7a}$$

$$=H(j\omega I-F)^{-1}PH^T+HP(-j\omega I-F^T)^{-1}H^T \tag{7b}$$

[Of course, straightforward discrete-time analogs of Eqs. (6) and (7) also exist.] In the above, P is required to be the positive semidefinite solution to the following steady-state Lyapunov equation:

$$FP+PF^T=-GQG^T \tag{8}$$

and

$$E[x(t)x^T(t)]=P \tag{9}$$

However, Ref. 28 implicitly considers the case above only when a positive semidefinite solution to Eq. (8) is *assumed* to exist, rather than invoking explicit conditions (as discussed below) that are necessary and sufficient to guarantee that solutions *do* exist. This absence of conditions for prescribing P to be positive semidefinite in what corresponds to Eq. (8) as it appears in Ref. 28 is somewhat paradoxical since another section of Ref. 28 (pp. 65–80) provides one of the most succinct expositions on the existence and uniqueness of positive definite/semidefinite solutions to the somewhat related Riccati equation.

Both the time- and frequency-domain expressions of Eqs. (6) and (7), respectively, are undefined (i.e., meaningless) unless Eq. (8) has both a unique *and* positive semidefinite solution. A unique solution is guaranteed to exist (see Ref. 27, lemma 1.5, p. 103; Ref. 24; and Ref. 30, Chap. 6) if and only if

$$F \text{ is strictly stable (i.e., } all \text{ eigenvalues have only negative real parts)} \tag{10}$$

and, additionally, the solution of Eq. (8) is guaranteed (Ref. 31, pp. 173–174 c.f., Ref. 26, p. 198) to be positive *semidefinite* by

$$(F,L^T) \text{ being a controllable pair} \tag{11}$$

where L is obtained from the following matrix factorization (e.g., as from a Choleski decomposition[33,34]) on the right-hand side of Eq. (12) as obtained from the computed matrix product on the left-hand side as

$$GQG^T=LL^T \tag{12}$$

Theoretically, a Choleski factorization of the above type can be performed only if GQG^T is positive definite (which is the case if both Q is positive definite *and* G is of full rank). Because it enjoys such renown for being exacting on topics relating to estimation, the presentation in Ref. 28 corresponding to Eqs. (6–8) has apparently been widely disseminated, unfortunately, without the explicit cautionary conditions of Eqs. (10–12) for when a positive semidefinite solution to Eq. (8) does in fact exist.

Thus, in applications of Kalman filtering, optimal feedback regulation/control, and Kalman filter measurement schedule optimization (see Ref. 38; Ref. 39, sect. 3; and Ref. 40 involving coupled Riccati and Lyapunov equations in a two-point boundary value problem) in investigating stability of linear systems via Lyapunov function techniques (Ref. 17), in representing the second-order statistics of time-invariant linear systems in either the time or frequency domain as occurs in validly using shaping filters (Ref. 46), and even in multi-channel spectral estimation (Ref. 45), a need frequently arises (as indicated above) to check the adequacy of square symmetric matrix solutions for positive definiteness/semidefiniteness. To achieve this, it is sometimes enough to just check the initial condition of Eq. (2) for positive definiteness (such as is done in navigation alignment applications involving a nondiagonal initial condition) if controllability/observability or weaker detectability/stabilizability of the system are already established to guarantee theoretically that the subsequent solution evolving as a function of time is positive definite. Other applications or algorithm implementations require intermediate checks on the adequacy of the solution in terms of being positive definite, since roundoff and truncation errors or the effects of approximations invoked can sometimes build up to eventually cause numerical difficulties. Reference 32 provides four lucid examples of how such deleterious situations can occur in even simple, apparently straightforward estimation applications. Thus, the third purpose of this Note is satisfied.

Practical Computational Tests

Although the Choleski decomposition (an algorithm of order n^3) is sometimes employed as a test for positive definiteness for large-dimensioned matrices, it is not totally satisfactory for that purpose. For a large nondiagonal matrix, one does not realistically know beforehand whether the matrix being tested for adequacy in an application is, in fact, positive definite, positive semidefinite, or neither. A symmetric matrix being positive definite is theoretically sufficient to guarantee that a Choleski factorization [such as that assumed to be used to extract L in Eq. (12)] can be accomplished (see Ref. 33, p. 263 and Ref. 34, p. 89). This further suggests that a likely computational approach for demonstrating positive definiteness is to attempt a Choleski factorization on a matrix and, if successfully carried to completion, the indication would be that the original matrix was positive definite. However, due to the effects of having finite bit-size registers in the computer and the consequent roundoff and truncation errors incurred, there are nonpathological cases (such as example 5.2-2 of Ref. 34) where a Choleski factorization fails to go to completion by encountering the square root of a negative number in what should be all-real arithmetic, even though the original matrix is positive definite. Thus, Choleski decomposition is not satisfactory as a test unless the definition of positive definiteness is amended to be "positive definite for all practical purposes on the particular machine with the particular precision" as a veritable Pandora's box.

Much less controversial would be to use the singular-value decomposition (SVD, as discussed in Sec. 3 of Ref. 35), as is recommended here as the proper method to reveal the fine distinctions of a matrix's positive definiteness or positive semidefiniteness in a way that correctly accounts for limits in the precision of a particular machine. The computational burden of an SVD is comparable to that of a Choleski factorization and validated SVD routines are available commercially in LINPACK or EISPACK (as indicated to be preferred implementations in Ref. 36, p. 167) and in IMSL. Even more efficient implementations of SVD using systolic arrays[37] are on the technical horizon to improve further its efficiency and speed as a practical computational test for both positive definiteness and positive semidefiniteness.

Conclusions

Recapitulating, the "principal minor test" for matrix positive semidefiniteness was re-examined here and pointers were provided to both correct and incorrect published versions of it as a cautionary reminder of what expert opinions to, respectively, either embrace or avoid on this subject. A brief review was provided of how important such tests are in applications involving matrix Riccati or Lyapunov equations that span many major developments in modern control and estimation theory. A few theorems/lemmas were reviewed that put in proper perspective the theoretical underpinnings of when Riccati and Lyapunov equations are to have positive definite and positive semidefinite solutions, respectively, and pointers were provided to practical examples from applications that present a problem in this regard. Limitations inherent in the "principal minor test" that prevent it from serving as the basis of a practical computer-based computational procedure for determining positive semidefiniteness were discussed and use of the Choleski decomposition (as had been previously recommended for that purpose) was also dismissed here on the grounds of technical incompatibility. However, the singular-value decomposition (SVD) is consistent with use of finite bit-size registers and limited-precision computers (as encountered in practice) and so is recommended here as the preferred test to be used for determining either matrix positive definiteness or semidefiniteness in a completely rigorous fashion. Additionally, alternative implementations of SVD are readily available for testing even relatively high-dimensional matrices (e.g., $n \geq 75$) that frequently arise in realistic industrial applications.

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Symmetric Kinematic Transformation Pair Using Euler Parameters

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THIS Note derives a kinematic transformation using Euler parameters (quaternion elements), which results in a symmetric pair of direct and inverse transformations. The construction of direction cosine matrices is not required, nor do the formulations depend upon quaternion algebra. While quaternion transformations offer several computational advantages[1,2] over direction cosines, the rather obscure algebra of hyperimaginary numbers hinders the analytic treatment of individual vector components.

In the method described here, a three-vector whose components are to be expressed in either of two orthogonal basis sets will be replaced by a four-vector in order to achieve the simple symmetry in the transformations. Both Kane[3] and Morton[4] have shown the advantages of using four-vector representations of certain quantities in dynamics. The transformation presented here facilitates these methods of analysis by eliminating the need to revert temporarily to three-vectors during coordinate transformation.

If A and B are two coordinate systems defined by dextral, orthonormal triads $(\boldsymbol{a}_1,\boldsymbol{a}_2,\boldsymbol{a}_3)$ and $(\boldsymbol{b}_1,\boldsymbol{b}_2,\boldsymbol{b}_3)$ respectively, and if the orientation of B relative to A is such that a rotation of A in the right-hand sense about the direction defined by the unit vector λ by an amount θ causes the $\boldsymbol{a}_j$ vectors to become parallel to the respective $\boldsymbol{b}_i$ vectors, then the orientation of B relative to A can be expressed by the use of the direction cosine matrix (DCM) C as

$$\boldsymbol{b}=C\boldsymbol{a} \tag{1}$$

where $\boldsymbol{a}=[\boldsymbol{a}_1,\boldsymbol{a}_2,\boldsymbol{a}_3]^T$ and $\boldsymbol{b}=[\boldsymbol{b}_1,\boldsymbol{b}_2,\boldsymbol{b}_3]^T$ and the elements of C are computed from the Euler parameters

$$\epsilon_1 \triangleq \lambda_1 \sin\frac{\theta}{2} \tag{2a}$$

$$\epsilon_2 \triangleq \lambda_2 \sin\frac{\theta}{2} \tag{2b}$$

$$\epsilon_3 \triangleq \lambda_3 \sin\frac{\theta}{2} \tag{2c}$$

$$\epsilon_4 \triangleq \cos\frac{\theta}{2} \tag{2d}$$

where $\lambda_i=\lambda\cdot\boldsymbol{a}_i=\lambda\cdot\boldsymbol{b}_i$, with the result (c.f. Ref. 3) that

$$\boldsymbol{b}_1=(\epsilon_1^2-\epsilon_2^2-\epsilon_3^2+\epsilon_4^2)\boldsymbol{a}_1+2(\epsilon_1\epsilon_2+\epsilon_3\epsilon_4)\boldsymbol{a}_2+2(\epsilon_3\epsilon_1-\epsilon_4\epsilon_2)\boldsymbol{a}_3 \tag{3}$$

Using the normalization constraint on the Euler parameters

$$\epsilon_1^2+\epsilon_2^2+\epsilon_3^2+\epsilon_4^2=1 \tag{4}$$

to eliminate the negative terms ϵ_2^2 and ϵ_3^2 from the first part in Eq. (3) yields

$$\boldsymbol{b}_1=-\boldsymbol{a}_1+2[(\epsilon_4^2+\epsilon_1^2)\boldsymbol{a}_1+(\epsilon_1\epsilon_2+\epsilon_4\epsilon_3)\boldsymbol{a}_2+(\epsilon_3\epsilon_1-\epsilon_4\epsilon_2)\boldsymbol{a}_3] \tag{5}$$

Similarly,

$$\boldsymbol{b}_2=-\boldsymbol{a}_2+2[(\epsilon_1\epsilon_2-\epsilon_4\epsilon_3)\boldsymbol{a}_1+(\epsilon_4^2+\epsilon_2^2)\boldsymbol{a}_2+(\epsilon_2\epsilon_3+\epsilon_4\epsilon_1)\boldsymbol{a}_3] \tag{6}$$

$$\boldsymbol{b}_3=-\boldsymbol{a}_3+2[(\epsilon_1\epsilon_3+\epsilon_4\epsilon_2)\boldsymbol{a}_1+(\epsilon_2\epsilon_3-\epsilon_4\epsilon_1)\boldsymbol{a}_2+(\epsilon_4^2+\epsilon_3^2)\boldsymbol{a}_3] \tag{7}$$

In matrix form, Eqs. (5–7) become

$$\boldsymbol{b}=-\boldsymbol{a}+2(E'+\epsilon_4\epsilon')\boldsymbol{a}=C\boldsymbol{a} \tag{8}$$

with

$$E'=\begin{bmatrix}\epsilon_1^2 & \epsilon_1\epsilon_2 & \epsilon_1\epsilon_3\\ \epsilon_2\epsilon_1 & \epsilon_2^2 & \epsilon_2\epsilon_3\\ \epsilon_3\epsilon_1 & \epsilon_3\epsilon_2 & \epsilon_3^2\end{bmatrix} \tag{9}$$

$$\epsilon'=\begin{bmatrix}\epsilon_4 & \epsilon_3 & -\epsilon_2\\ -\epsilon_3 & \epsilon_4 & \epsilon_1\\ \epsilon_2 & \epsilon_1 & \epsilon_4\end{bmatrix} \tag{10}$$

It should be noted that Eq. (8) is formally somewhat similar to Eqs. (12–13b) in Ref. 1 and that it contains the same information as Eq. (21) on p. 14 of Ref. 3; however, there is an important symmetry in Eq. (8) (obtained by eliminating the negative quadratic terms in the Euler parameters rather than the positive ones) that will be exploited later. By augmenting the matrices E' and ϵ' with an extra row and column, some additional symmetry is achieved. Define the 4×4 matrices

$$E\triangleq\beta\beta^T \tag{11}$$

where

$$\beta=[\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4]^T \tag{12}$$

$$R\triangleq\begin{bmatrix}\epsilon_4 & \epsilon_3 & -\epsilon_2 & \epsilon_1\\ -\epsilon_3 & \epsilon_4 & \epsilon_1 & \epsilon_2\\ \epsilon_2 & -\epsilon_1 & \epsilon_4 & \epsilon_3\\ -\epsilon_1 & -\epsilon_2 & -\epsilon_3 & \epsilon_4\end{bmatrix} \tag{13}$$

Letting

$$\boldsymbol{a}^*=[\boldsymbol{a}_1,\boldsymbol{a}_2,\boldsymbol{a}_3,0]^T \tag{14a}$$

$$\boldsymbol{b}^*=[\boldsymbol{b}_1,\boldsymbol{b}_2,\boldsymbol{b}_3,0]^T \tag{14b}$$

gives

$$\boldsymbol{b}^*=-\boldsymbol{a}^*+2(E+\epsilon_4 R)\boldsymbol{a}^*=C^*\boldsymbol{a}^* \tag{15}$$

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