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OF A  $3 \times 3$  POSITIVE DEFINITE MATRIX**

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## ABSTRACT

An efficient closed form to compute the square root of a  $3 \times 3$  positive definite matrix is presented. The derivation employs the Cayley-Hamilton theorem avoiding calculation of eigenvectors. We show that evaluation of one eigenvalue of the square root matrix is needed and can not be circumvented. The algorithm is robust and efficient.

## RESUMO

Uma forma fechada eficiente para computar a raiz quadrada de uma matriz positiva definida  $3 \times 3$  é apresentada. A derivação emprega o teorema de Cayley-Hamilton evitando o cálculo de autovetores. Nós mostramos que a avaliação de um autovalor da matriz raiz quadrada é necessária e não pode ser evitado. O algoritmo é robusto e eficiente.

## 1. Introduction

The computation of the square root of a  $3 \times 3$  positive definite matrix plays an important role in an increasing number of applications. In the study of finite deformation applied, for example, to nonlinear shell analysis, as part of the overall solution process, the stretch tensor ( $U$ ) has to be computed from its square, the strain tensor ( $C$ ). This computation may be stated as: given a positive definite matrix  $C$ , compute  $U$  (and maybe  $U^{-1}$  as well) such that,

$$U^2 = C. \quad (1)$$

This computation is repeated in each element of a domain discretization and may quickly drive CPU costs up as the size of the problem increases. Therefore, the pursuit of strategies to efficiently compute  $U$  is of practical concern.

The first step in this direction, as far as we are aware of, was taken by Marsden and Hughes [1983], p. 55. They showed that a direct computation of  $U$  is possible employing the Cayley-Hamilton theorem, circumventing the usual expensive procedure of solving the eigenvalue problem for  $C$ . They have worked out explicit formulae for the  $2 \times 2$  case, and, independently, Hoger and Carlson [1984] systematically derived formulas for this and the  $3 \times 3$  cases. For the  $3 \times 3$  case, Hoger and Carlson showed that the problem is transferred to finding a solution of a quartic equation on the first invariant of  $U$ . In selecting a solution for this equation, they argued uniqueness of a positive root, possibility which does not hold in general, as observed by Sawyers [1986]. As an alternative, Sawyers suggested that the first invariant of  $U$  be computed directly from its eigenvalues, which in turn are calculated from the characteristic equation of  $C$ , a cubic equation in the square of each eigenvalue of  $U$ . The remainder of the procedure constitutes direct application of the formulas derived by Hoger and Carlson. This alternative had already been introduced by Stephenson [1983]

in a unpublished work.

In this paper we show the existence of an algorithm emanating from Hoger and Carlson's approach. We show that the quartic equation on the first invariant of  $U$  alluded above is intimately linked to the solution of the characteristic equation of  $C$ . This algebraic fact allows us to select the correct invariant solution of the quartic equation out of the four possible roots. The resulting algorithm depends on the computation of *one* eigenvalue of  $U$  (not on *all* of them!) and from the explicit expressions of the eigenvalues, given by Stephenson/Sawyers, we select the largest one. In practice, this procedure has proven to be more robust than the Stephenson/Sawyers's alternative, and examples are presented in appendix 1 to support this evidence. Also, the computational effort involved in the present algorithm is about the same as Stephenson/Sawyers option.

Throughout we denote by  $\lambda_i$  ( $i = 1, \dots, n_{sd}$ ) the eigenvalues of  $U$  and, consequently, by  $\lambda_i^2$  the corresponding eigenvalues of  $C$ . Here  $n_{sd}$  is the dimension of the problem (2 or 3 in this paper). We reserve the symbol  $I$  for the identity matrix with entries

$$I_{ij} = \delta_{ij}, \quad i, j = 1, \dots, n_{sd} \quad (2)$$

where  $\delta_{ij}$  is the Kronecker delta.

An outline follows. In Section 2 we solve the  $2 \times 2$  case as a model for the  $3 \times 3$  case presented in Section 3. Some concluding remarks are drawn in Section 4.

Before proceeding, we should also mention that Ting [1985] studied the same problem and extensions to other isotropic tensor functions using the representation theorem of Serrin [1959], but did not address the algebra involved in the determination of the invariants of  $U$ . Morman [1986] has also investigated isotropic tensor functions along similar lines as Ting, and his solution also depends on the computation of all eigenvalues of  $C$  as in

Stephenson/Sawyers.

## 2. Two-Dimensional Case

In this section we lay out steps to obtain  $U$  and  $U^{-1}$  from  $C$ , a  $2 \times 2$  matrix. The same methodology applies to the  $3 \times 3$  case.

Let us first introduce the principal invariants of  $U$ ,

$$I_U = \text{tr } U = \lambda_1 + \lambda_2$$

$$II_U = \det U = \lambda_1 \lambda_2 \quad (3)$$

By the Cayley-Hamilton theorem,

$$U^2 - I_U U + II_U I = 0 \quad (4)$$

Using (1), we can solve (4) for  $U$ ,

$$U = \frac{1}{I_U} (II_U I + C) \quad (5)$$

If we multiply (4) by  $U^{-1}$  we obtain

$$U^{-1} = \frac{1}{II_U} (I_U I - U) \quad (6)$$

and by employing (5),

$$U^{-1} = \frac{1}{I_U II_U} ((I_U^2 - II_U) I - C) \quad (7)$$

In order to apply (5) and (7) we need to relate the invariants of  $U$  to the invariants of  $C$ ,

$$I_C = \text{tr } C = \lambda_1^2 + \lambda_2^2,$$

$$II_C = \det C = \lambda_1^2 \lambda_2^2. \quad (8)$$

Comparing (3) and (8)

$$\begin{aligned} I_C &= I_U^2 - 2II_U \\ II_C &= II_U^2 \end{aligned} \tag{9}$$

and therefore,

$$\begin{aligned} II_U &= \sqrt{II_C} \\ I_U &= \sqrt{I_C + 2\sqrt{II_C}} \end{aligned} \tag{10}$$

**Remark**

We adapted the presentation by Ting [1985] in the determination of  $U$  and  $U^{-1}$  as in equations (5) and (7). A similar observation applies to the next section. However, Ting did not address how to compute the invariants of  $U$ , fundamental to the solution of the problem.

**3. Three-Dimensional Case** (or solution set to Problem 3.3 of Marsden and Hughes [1983], pg. 55)

Proceeding as in the last section, introduce the principal invariants of  $U$ ,

$$\begin{aligned} I_U &= \text{tr } U = \lambda_1 + \lambda_2 + \lambda_3 \\ II_U &= \frac{1}{2} [(\text{tr } U)^2 - \text{tr}(U^2)] = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 \end{aligned} \tag{11}$$

$$III_U = \det U = \lambda_1\lambda_2\lambda_3$$

Again, by the Cayley-Hamilton theorem,

$$U^3 - I_U U^2 + II_U U - III_U I = 0 \tag{12}$$

which when multiplied by  $U$  gives

$$U^4 - I_U U^3 + II_U U^2 - III_U U = 0 \quad (13)$$

We now substitute  $U^3$  from (12) into (13) and repeatedly use (1) to obtain,

$$U = \frac{1}{I_U II_U - III_U} [I_U III_U I + (I_U^2 - II_U)C - C^2] \quad (14)$$

By multiplying (12) by  $U^{-1}$  we obtain

$$U^{-1} = \frac{1}{III_U} (II_U I - I_U U + C) \quad (15)$$

and using (14),

$$U^{-1} = \frac{1}{III_U (I_U II_U - III_U)} [(I_U II_U^2 - III_U (I_U^2 + II_U))I - (III_U + I_U (I_U^2 - 2II_U))C + I_U C^2] \quad (16)$$

The calculation of the invariants of  $U$  in terms of the invariants of  $C$  is now more elaborate and the derivation of the appropriate expressions will take all the rest of this section.

The invariants of  $C$  are

$$\begin{aligned} I_C &= \text{tr } C = \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \\ II_C &= \frac{1}{2} [(\text{tr } C)^2 - \text{tr } (C^2)] = \lambda_1^2 \lambda_2^2 + \lambda_1^2 \lambda_3^2 + \lambda_2^2 \lambda_3^2 \\ III_C &= \det C = \lambda_1^2 \lambda_2^2 \lambda_3^2. \end{aligned} \quad (17)$$

Comparing (11) and (17)

$$I_C = I_U^2 - 2II_U$$



$$II_C = II_U^2 - 2I_U III_U \quad (18)$$

$$III_C = III_U^2$$

and therefore,

$$III_U = \sqrt{III_C}$$

$$I_U^2 = I_C + 2II_U \quad (19)$$

$$II_U^2 = II_C + 2\sqrt{III_C}I_U$$

Solving for  $I_U$  in the last two equations yields

$$I_U^4 - 2I_C I_U^2 - 8\sqrt{III_C}I_U + I_C^2 - 4II_C = 0 \quad (20)$$

This is the quartic equation in  $I_U$  obtained by Hoger and Carlson [1984]. Sawyers [1986] gave an explicit example with distinct positive roots, possibility ruled out by Hoger and Carlson. This led Sawyers to compute the eigenvalues of  $C$  (to determine directly the invariants of  $U$ ). This can be done by solving the characteristic equation for  $\lambda^2$ :

$$\lambda^6 - I_C \lambda^4 + II_C \lambda^2 - III_C = 0 \quad (21)$$

We go back to the quartic equation of Hoger and Carlson and show how to select the correct root out of the four possible ones. First note that the quartic equation can be split into two quadratics (standard in solving quartic equations, see e.g., Dobbs and Hanks [1980]):

$$\begin{aligned} 0 &= I_U^4 - 2I_C I_U^2 - 8\sqrt{III_C}I_U + I_C^2 - 4II_C = \\ &= (I_U^2 + mI_U + n)(I_U^2 - mI_U + p) \end{aligned} \quad (22)$$

Equating coefficients yields,

$$n = \frac{m^3 - 2I_C m + 8\sqrt{III_C}}{2m} \quad (23)$$

$$p = m^2 - 2I_C - n = \frac{m^3 - 2I_C m - 8\sqrt{III_C}}{2m} \quad (24)$$

and a cubic equation in  $m^2$ ,

$$m^6 - 4I_C m^4 + 16III_C m^2 - 64IIIC = 0 \quad (25)$$

Dividing this last equation by 64 reproduces (21) with

$$\frac{m^2}{4} = \lambda^2 \quad (26)$$

or restricting to the positive value of  $m$ ,

$$m = 2\lambda. \quad (27)$$

This is an interesting result: *each positive root of (25) is a multiple of each positive root of (21)*. Based on this knowledge we will be able to single out the meaningful root of the quartic (20). Let us write the four roots. From (22),

$$I_U = \begin{cases} \frac{-m \pm \sqrt{m^2 - 4n}}{2} \\ \frac{m \pm \sqrt{m^2 - 4p}}{2} \end{cases} \quad (28)$$

Using (23), (24) and (27) gives

$$I_U = \begin{cases} -\lambda \pm \sqrt{\frac{-\lambda^3 + I_C \lambda - 2\sqrt{III_C}}{\lambda}} \\ \lambda \pm \sqrt{\frac{-\lambda^3 + I_C \lambda + 2\sqrt{III_C}}{\lambda}} \end{cases} \quad (29)$$

To examine (29) further substitute  $\lambda$  by any of the positive eigenvalues  $\lambda_1, \lambda_2$  or  $\lambda_3$ , the definition of  $I_C$  and  $III_C$  from eq. (17) to get,

$$I_U = \begin{cases} -\lambda_1 + \lambda_2 - \lambda_3 \\ -\lambda_1 - \lambda_2 + \lambda_3 \\ \lambda_1 + \lambda_2 + \lambda_3 \\ \lambda_1 - \lambda_2 - \lambda_3 \end{cases} \quad (30)$$

Thus, the definition of  $I_U$  corresponds to the third root and the desired solution is

$$I_U = \lambda + \sqrt{\frac{-\lambda^3 + I_C \lambda + 2\sqrt{III_C}}{\lambda}} \quad (31)$$

To complete our task we need to compute one of the eigenvalues  $\lambda$ , a positive root of (21). We will do it in detail to illustrate degenerate cases. <sup>(1)</sup> We take advantage of the fact that all the roots are real (actually they are all positive in  $\lambda^2$ ), and use standard algebraic manipulation appropriate to this particular case (see, e.g., Mathews [1971]).

First translate the solution to avoid the quadratic term

$$\lambda^2 = x + \frac{I_C}{3} \quad (32)$$

which transforms (21) into

$$x^3 + (III_C - \frac{I_C^2}{3})x - \frac{2}{27}I_C^3 + \frac{I_C III_C}{3} - III_C = 0 \quad (33)$$

Note that

$$k = I_C^2 - 3III_C = \frac{1}{2}[(\lambda_1^2 - \lambda_2^2)^2 + (\lambda_1^2 - \lambda_3^2)^2 + (\lambda_2^2 - \lambda_3^2)^2] \geq 0 \quad (34)$$

---

<sup>(1)</sup> The following discussion is based upon Stephenson [1983]. Sawyers [1986] presented the same final solution *modulo* the isotropic degenerate case.

and is equal to zero only if  $C$  is isotropic. Assuming that  $C$  is not isotropic we can make the change of variables

$$y = \frac{3}{2}k^{-1/2}x \quad (35)$$

yielding for (33),

$$4y^3 - 3y = \frac{l}{k^{3/2}} \quad (36)$$

with

$$l = I_C^3 - \frac{9}{2}I_C II_C + \frac{27}{2}III_C. \quad (37)$$

From (34) and (37), after some algebra

$$1 - \frac{l^2}{k^3} = \frac{54(\lambda_1^2 - \lambda_2^2)^2(\lambda_1^2 - \lambda_3^2)^2(\lambda_2^2 - \lambda_3^2)^2}{[(\lambda_1^2 - \lambda_2^2)^2 + (\lambda_1^2 - \lambda_3^2)^2 + (\lambda_2^2 - \lambda_3^2)^2]^3} \geq 0 \quad (38)$$

and therefore

$$\left| \frac{l}{k^{3/2}} \right| \leq 1 \quad (39)$$

Introducing  $y = \cos \theta$ ,  $\frac{l}{k^{3/2}} = \cos \phi$  reduces (35) to

$$\cos 3\theta = \cos \phi \quad (40)$$

and thus

$$\theta_i = \frac{1}{3}(\phi + 2\pi(i-1)), \quad i = 1, 2, 3 \quad (41)$$

Combining (32) to (41) gives

$$\lambda_i^2 = \frac{1}{3} \{ I_C + 2k^{1/2} \cos[\frac{1}{3}(\phi + 2\pi(i-1))] \}, \quad i = 1, 2, 3 \quad (42)$$

with

$$\phi = \cos^{-1} \left[ \frac{2I_C^3 - 9I_C II_C + 27III_C}{2k^{3/2}} \right] \quad (43)$$

If  $C$  is isotropic ( $k = 0$ ) we alternatively use

$$\lambda = \lambda_i^2 = \frac{I_C}{3}, \quad i = 1, 2, 3 \quad (44)$$

and (14)-(15) reduce to

$$U = \lambda I, \quad U^{-1} = \lambda^{-1} I \quad (45)$$

For our purposes we just need one root of (42). We select  $i = 1$ , since this root gives the largest eigenvalue (according to the usual convention that  $\cos^{-1}$  has range over 0 to  $\pi$ ). This root is used in (31) to finally compute  $I_U$ . The other invariants of  $U$  are recovered from (19) and we are ready to use (14) and (16) to calculate  $U$  and  $U^{-1}$ . A flowchart illustrates the algorithm in Box 1.

#### Remarks

1. Having to calculate one eigenvalue of  $U$  poses a dilemma: why not calculate all of them using (42) (as suggested by R. Stephenson [1983] and K. Sawyers [1986])? The answer comes from a computational aspect: by only computing the largest eigenvalue results in a more robust algorithm than having to compute them all. This is of particular interest when small eigenvalues are involved and round-off may poison Stephenson/Sawyers procedure but not the present method (see appendix 1 for examples).
2. Ting [1985] has pointed out that the representation of  $U$  is not unique when we have two repeated eigenvalues (e.g.,  $\lambda_1 \neq \lambda_2 = \lambda_3$ ). There is no breakdown in the algorithm presented and the formulae in Box 1 can be used as one possible representation.

#### 4. Conclusions

Employing the Cayley-Hamilton theorem simplifies the determination of the square-root of a positive definite matrix ( $C^{1/2}$ ). Applying the methodology developed by Hoger

and Carlson to the  $3 \times 3$  matrix case, the problem reduces to a quartic equation in the first invariant of  $U = C^{1/2}$ . We showed that the solution of this equation can be unambiguously selected and it is dependent on the computation of *one* eigenvalue of  $U$ . The resulting algorithm is slightly simpler and has performed better than having to compute all eigenvalues of  $U$ .

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**Box 1. Algorithm to Compute  $U$  and/or  $U^{-1}$** **Step 1: Invariants of  $C$** 

$$I_C = \text{tr } C$$

$$II_C = \frac{1}{2} [I_C^2 - \text{tr}(C^2)]$$

$$III_C = \det C$$

$$k = I_C^3 - 3II_C$$

**Step 2: Isotropy check**

If ( $k \leq \text{tol}$ ) then

$$\lambda = \sqrt{\frac{I_C}{3}}$$

$$U = \lambda I$$

$$U^{-1} = \lambda^{-1} I$$

return

endif

**Step 3: Calculate largest eigenvalue**

$$l = I_C^3 \left( I_C - \frac{9}{2} II_C \right) + \frac{27}{2} III_C$$

$$\phi = \cos^{-1} \left[ \frac{l}{k^{3/2}} \right]$$

$$\lambda^2 = \frac{1}{3} \left\{ I_C + 2k^{1/2} \cos \left( \frac{\phi}{3} \right) \right\}$$

Step 4: Invariants of  $U$

$$III_U = \sqrt{III_C}$$

$$I_U = \lambda + \sqrt{-\lambda^2 + I_C + \frac{2III_U}{\lambda}}$$

$$II_U = \frac{I_U^2 - I_C}{2}$$

Step 5:  $U$  and  $U^{-1}$

$$U = \frac{1}{I_U II_U - III_U} [I_U III_U I + (I_U^2 - II_U)C - C^2]$$

$$U^{-1} = \frac{1}{III_U} (II_U I - I_U U + C)$$

return

end

**Box 2. Stephenson/Sawyers alternative**

Replace steps 3 and 4 of algorithm in Box 1 by:

**Step 3:** Compute all eigenvalues

$$l = I_C^2 \left( I_C - \frac{9}{2} II_C \right) + \frac{27}{2} III_C$$

$$\phi = \cos^{-1} \left[ \frac{l}{k^{3/2}} \right]$$

$$\cos \theta_1 = \cos \left( \frac{\phi}{3} \right)$$

$$\sin \theta_1 = \sqrt{1 - (\cos \theta_1)^2}$$

$$\cos \theta_2 = -(\cos \theta_1 + \sqrt{3} \sin \theta_1)/2$$

$$\cos \theta_3 = -(\cos \theta_1 - \sqrt{3} \sin \theta_1)/2$$

$$\lambda_1^2 = \frac{1}{3} \{ I_C + 2k^{1/2} \cos \theta_1 \}$$

$$\lambda_2^2 = \frac{1}{3} \{ I_C + 2k^{1/2} \cos \theta_2 \}$$

$$\lambda_3^2 = \frac{1}{3} \{ I_C + 2k^{1/2} \cos \theta_3 \}$$

**Step 4:** Invariants of  $U$

$$I_U = \lambda_1 + \lambda_2 + \lambda_3$$

$$II_U = \lambda_1(\lambda_2 + \lambda_3) + \lambda_2\lambda_3$$

$$III_U = \lambda_1\lambda_2\lambda_3$$

### Appendix 1: Numerical experiments

In this appendix we compare the method proposed (Box 1) with Stephenson/Sawyers alternative (Box 2). To assess the robustness with respect to the influence of round-off errors, both methodologies were programmed in single precision.

As a simple example consider,

$$C = \text{diag}(2 + \epsilon, 1 + \epsilon, \epsilon)$$

then, for this case,  $U = C^{1/2}$  follows immediately

$$U = \text{diag}(\sqrt{2 + \epsilon}, \sqrt{1 + \epsilon}, \sqrt{\epsilon})$$

In the table below we compare the exact computation of  $\lambda_3 = \sqrt{\epsilon}$  with the results using each method for different values of  $\epsilon$  (no difference was observed in the computations of  $\lambda_1$  and  $\lambda_2$ ). As  $\epsilon \rightarrow 0$  the results employing Stephenson/Sawyers alternative quickly deteriorates. Although this example is deceptively simple, it is illustrative of the behavior of both algorithms when applied to matrices with small eigenvalues.

$\epsilon$	Exact = $\sqrt{\epsilon}$	Present method	Stephenson/Sawyers
0.01	0.1	0.09999998	0.1000002
0.0001	0.01	0.009999998	0.01000371
0.000001	0.001	0.001000000	0.0009766223
0.0000001	0.0003162278	0.0003162278	0.0000001292893

As a more interesting example take

$$C = \begin{pmatrix} 400.0 & 0. & 0. \\ & 0.9999000 & 0.009998333 \\ \text{symm} & & 0.0001999867 \end{pmatrix}.$$

The exact value of  $U$  up to seven significant digits is

$$U = \begin{pmatrix} 20.00000 & 0. & 0. \\ & 0.9999010 & 0.009899340 \\ \text{symm} & & 0.01009900 \end{pmatrix}.$$

Employing the method in Box 1 we obtain

$$U = \begin{pmatrix} 20.00003 & 0. & 0. \\ & 0.9999052 & 0.009899381 \\ \text{symm} & & 0.01009904 \end{pmatrix},$$

and by Stephenson/Sawyers alternative

$$U = \begin{pmatrix} 20.00003 & 0. & 0. \\ & 1.001076 & 0.009513555 \\ \text{symm} & & 0.04984753 \end{pmatrix}.$$

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