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A recursion formula for the integer power of a symmetric second-order tensor and its application to computational plasticity

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Summary. In this paper, a recursion formula is given for the integer power of a second-order tensor in 3D Euclidean space. It can be used in constitutive modelling for approximating failure or yield surfaces with corners and it is demonstrated for the case of Rankine failure criterion. Removing corners provides clear advantages in computational plasticity. We discuss the consequences of the approximation errors for failure analyses of brittle and quasi-brittle materials.

Key words: second order tensor, recursion formula, Cayley-Hamilton equation, Rankine failure criterion

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In memory of our friends Dr Djebar Baroudi and Lic.Tech. Jari Laukkanen

Introduction

In computational plasticity yield surface corners produce non-uniqueness in the plastic flow direction if associative flow rule is applied. Koiter built a theoretical framework for corner plasticity [6, 7, 10]. In computational framework it has resulted in numerous studies and also many approaximate expressions for multi-surface yield surfaces with corners have been presented, see e.g. [1, 2, 12, 13, 14]. Similar problem arises in continuum damage mechanics, especially when it is formulated in terms of the maximum principal stress, like in the classic Rankine failure criterion, which is linear in the principal stress space but non-linear in the global stress space [3]. Approximation of such yield/failure surfaces with a continuous function written in terms of the stress invariants offers clear advantages since it does not involve solution of the principal stresses and coordinate transformations. Moreover, the consistent linearization needed in the implicit integration schemes is straightforward.

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Scalar invariants of a second order symmetric tensor

The characteristic equation for the solution of the eigenvalues λ of a symmetric second-order tensor $\mathbf{A}$ in a three-dimensional Euclidean space is

$$-\lambda^3 + I_1\lambda^2 + I_2\lambda + I_3 = 0, \tag{1}$$

where the principal scalar invariants I_i, $i = 1, 2, 3$ of the tensor $\mathbf{A}$ are defined as

$$I_1 = \operatorname{tr}\mathbf{A} = A_{ii}, \tag{2}$$
$$I_2 = \tfrac{1}{2}\left[\operatorname{tr}(\mathbf{A}^2) - (\operatorname{tr}\mathbf{A})^2\right] = \tfrac{1}{2}(A_{ij}A_{ji} - A_{ii}A_{jj}), \tag{3}$$
$$I_3 = \det\mathbf{A} = \epsilon_{ijk}A_{1i}A_{2j}A_{3k}, \tag{4}$$

where ϵ_{ijk} is the permutation tensor and standard index notation is used. If the eigenvalues of $\mathbf{A}$ are denoted as λ_1, λ_2 and λ_3, the scalar invariants (2)–(3) can be expressed as

$$I_1 = \lambda_1 + \lambda_2 + \lambda_3, \tag{5}$$
$$I_2 = -\lambda_1\lambda_2 - \lambda_2\lambda_3 - \lambda_3\lambda_1, \tag{6}$$
$$I_3 = \lambda_1\lambda_2\lambda_3. \tag{7}$$

It should be noted that the definition of the scalar invariants of a tensor is not unique. In the literature, often the quadratic principal invariant is defined as the opposite sign, see e.g. [4, 9]. However, the authors prefer to express the invariants of a tensor and its deviator, which is extensively used in the plasticity theory, in a similar way. This convention is also adopted by Lubliner [8]. Further elaboration of the tensor invariants and characteristic equation can be found in [15, Sect. 8].

The well-known Cayley-Hamilton equation states that a tensor itself satisfies its characteristic equation

$$\mathbf{A}^3 = I_1\mathbf{A}^2 + I_2\mathbf{A} + I_3\mathbf{I}, \tag{8}$$

where $\mathbf{I}$ is the second order identity tensor. From (8) it can be easily deduced that the cubic invariant I_3 can also be expressed as

$$I_3 = \det\mathbf{A} = \tfrac{1}{3}\operatorname{tr}(\mathbf{A}^3) - \tfrac{1}{2}\operatorname{tr}\mathbf{A}\operatorname{tr}(\mathbf{A}^2) + \tfrac{1}{6}(\operatorname{tr}\mathbf{A})^3. \tag{9}$$

The recursion formula

To compute higher than third order powers of a tensor in 3D Euclidean space the following recursion formula can be proven. If n is a positive integer, $n \geq 1$, the power $\mathbf{A}^{3+n}$ can be computed as

$$\mathbf{A}^{3+n} = a_1^{(n)}\mathbf{A}^2 + a_2^{(n)}\mathbf{A} + a_3^{(n)}\mathbf{I}, \tag{10}$$

where the coefficients $a_i^{(n)}$, $i = 1, 2, 3$ are given by the recursion formulas

$$a_1^{(n)} = I_1 a_1^{(n-1)} + a_2^{(n-1)}, \tag{11}$$
$$a_2^{(n)} = I_2 a_1^{(n-1)} + a_3^{(n-1)}, \tag{12}$$
$$a_3^{(n)} = I_3 a_1^{(n-1)}, \tag{13}$$

with the initial values

$$a_1^{(0)} = I_1, \quad a_2^{(0)} = I_2, \quad a_3^{(0)} = I_3. \tag{14}$$

Proof

A proof for the above formula is given by mathematical induction.

1. The equation (10) is true for $n = 0$, i.e.

$$\mathbf{A}^3 = a_1^{(0)}\mathbf{A}^2 + a_2^{(0)}\mathbf{A} + a_3^{(0)}\mathbf{I} = I_1\mathbf{A}^2 + I_2\mathbf{A} + I_3\mathbf{I},$$

   which is the Cayley-Hamilton equation (8).
2. Assume that the equation holds for $n = k$. Then it has to be proved that it holds also for $n = k + 1$.

$$\begin{aligned}\mathbf{A}^{3+k+1} &= a_1^{(k+1)}\mathbf{A}^2 + a_2^{(k+1)}\mathbf{A} + a_3^{(k+1)}\mathbf{I} \\ &= (I_1 a_1^{(k-1)} + a_2^{(k-1)})\mathbf{A}^2 + (I_2 a_1^{(k-1)} + a_3^{(k-1)})\mathbf{A} + I_3 a_1^{(k)}\mathbf{I} \\ &= a_1^{(k)}(I_1\mathbf{A}^2 + I_2\mathbf{A} + I_3\mathbf{I}) + a_2^{(k)}\mathbf{A}^2 + a_3^{(k)}\mathbf{A} \\ &= a_1^{(k)}\mathbf{A}^3 + a_2^{(k)}\mathbf{A}^2 + a_3^{(k)}\mathbf{A} \\ &= (a_1^{(k)}\mathbf{A}^2 + a_2^{(k)}\mathbf{A} + a_3^{(k)}\mathbf{I})\mathbf{A} \\ &= \mathbf{A}^{3+k}\mathbf{A} = \mathbf{A}^{3+k+1}.\end{aligned}$$

It should be noted that $\mathbf{A}$ and its powers are coaxial, i.e. they have same eigenvectors, thus the product $\mathbf{A}^m\mathbf{A}$ is commutative, i.e. $\mathbf{A}^m\mathbf{A} = \mathbf{A}\mathbf{A}^m$.

An alternative derivation of the recurrence scheme can be found in [5, Section 7.5].

Some comments

It is clear that the above recursion formulas are valid also for a deviatoric tensor too. In such a case the linear invariant I_1 is identically zero in equations (11)–(13).

Constitutive models for isotropic solids are often expressed in terms of invariants I_1, J_2 and J_3 or I_1, J_2 and θ, where J_2 and J_3 are the quadratic and cubic invariants of the deviatoric tensor

$$\operatorname{dev}\mathbf{A} = \mathbf{A} - \tfrac{1}{3}I_1\mathbf{I}, \tag{15}$$

and θ is the Lode angle, which in the deviatoric plane can be determined from equation

$$\cos 3\theta = \frac{3\sqrt{3}}{2}\frac{J_3}{J_2^{3/2}}, \quad \text{where} \quad J_2 = \frac{1}{2}\operatorname{tr}(\operatorname{dev}\mathbf{A}), \quad J_3 = \det(\operatorname{dev}\mathbf{A}). \tag{16}$$

For example, in the case of stress tensor, i.e. $\mathbf{A} = \boldsymbol{\sigma}$, the invariants I_1, J_2 and θ have clear physical and geometrical meaning: I_1 is related to the mean stress $\sigma_{\mathrm{m}} = \frac{1}{3}I_1$ and also related to the length $\xi = |ON| = \sqrt{3}\sigma_{\mathrm{m}}$ on the hydrostatic axis, J_2 to the magnitude of the deviatoric stress $\rho = \sqrt{2J_2}$ and θ gives the orientation on the deviatoric plane, see figure 1b. The coordinates ξ, ρ and θ are called the Haigh-Westergaard stress space coordinates.

Naturally, the invariants I_2 and I_3 can be expressed in terms of invariants I_1, J_2 and J_3 as

$$I_2 = J_2 - \tfrac{1}{3}I_1^2, \qquad I_3 = J_3 - \tfrac{1}{3}I_1 J_2 + \tfrac{1}{27}I_1^3. \tag{17}$$

Many times it is convenient to express invariants I_1 and J_2 in terms of mean stress $\sigma_{\mathrm{m}} = \frac{1}{3}I_1$ and effective stress $\sigma_{\mathrm{e}} = \sqrt{3J_2}$. With these definitions, expressions (17) can be written as

$$I_2 = \tfrac{1}{3}\sigma_{\mathrm{e}}^2 - 3\sigma_{\mathrm{m}}^2, \qquad I_3 = J_3 - \tfrac{1}{3}\sigma_{\mathrm{m}}\sigma_{\mathrm{e}}^2 + \sigma_{\mathrm{m}}^3. \tag{18}$$

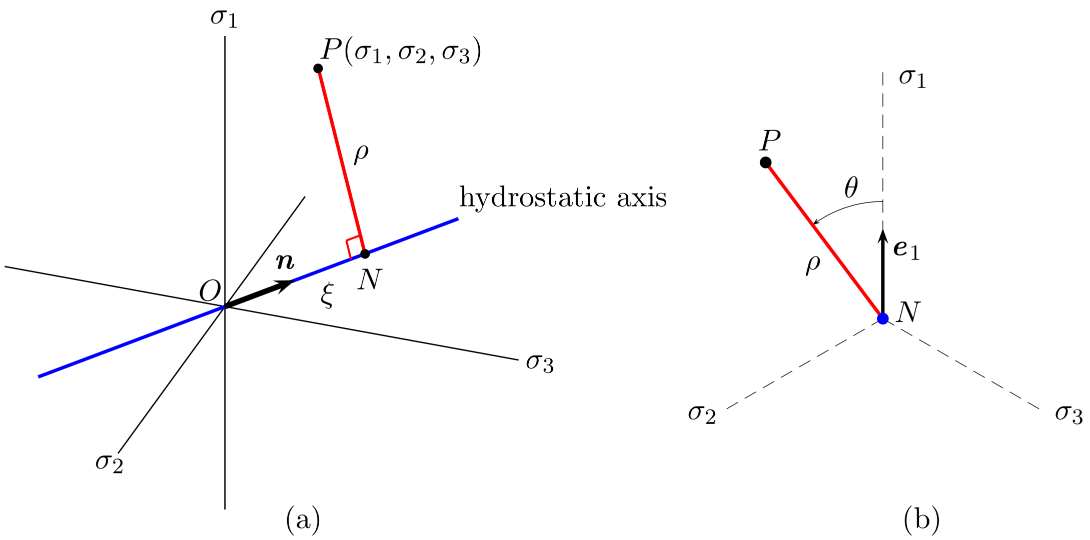


Figure 1. (a) Principal stress space. (b) Deviatoric plane. The projections of the principal stress axes are shown with dashed line.

Taking (16) into account the third stress invariant has the form

$$I_3 = \tfrac{2}{27}\sigma_{\mathrm{e}}^3 \cos 3\theta - \tfrac{1}{3}\sigma_{\mathrm{m}}\sigma_{\mathrm{e}}^2 + \sigma_{\mathrm{m}}^3. \tag{19}$$

Examples

As an illustration, some first higher order powers are given. The powers $\mathbf{A}^4, \mathbf{A}^5$ and $\mathbf{A}^6$ are

$$\begin{aligned}\mathbf{A}^4 &= a_1^{(1)}\mathbf{A}^2 + a_2^{(1)}\mathbf{A} + a_3^{(1)}\mathbf{I}\\ &= (I_1^2 + I_2)\mathbf{A}^2 + (I_1 I_2 + I_3)\mathbf{A} + I_1 I_3\mathbf{I},\end{aligned} \tag{20}$$

$$\begin{aligned}\mathbf{A}^5 &= a_1^{(2)}\mathbf{A}^2 + a_2^{(2)}\mathbf{A} + a_3^{(2)}\mathbf{I}\\ &= (I_1 a_1^{(1)} + a_2^{(1)})\mathbf{A}^2 + (I_2 a_1^{(1)} + a_3^{(1)})\mathbf{A} + I_3 a_1^{(1)}\mathbf{I}\\ &= (I_1^3 + 2I_1 I_2 + I_3)\mathbf{A}^2 + (I_2^2 + I_1^2 I_2 + I_1 I_3)\mathbf{A} + (I_1^2 + I_2)I_3\mathbf{I},\end{aligned} \tag{21}$$

$$\begin{aligned}\mathbf{A}^6 &= a_1^{(3)}\mathbf{A}^2 + a_2^{(3)}\mathbf{A} + a_3^{(3)}\mathbf{I}\\ &= (I_1 a_1^{(2)} + a_2^{(2)})\mathbf{A}^2 + (I_2 a_1^{(2)} + a_3^{(2)})\mathbf{A} + I_3 a_1^{(2)}\mathbf{I}\\ &= (I_1^4 + 3I_1^2 I_2 + I_2^2 + 2I_1 I_3)\mathbf{A}^2 + \left[(I_1^3 + 2I_1 I_2 + I_3)I_2 + (I_1^2 + I_2)I_3\right]\mathbf{A} +\\ &\quad + (I_1^3 + 2I_1 I_2 + I_3)I_3\mathbf{I}.\end{aligned} \tag{22}$$

Application

Applications for higher-order powers of a tensor can be found in constitutive models to round corners in yield and/or failure surfaces. A simple example is a Rankine-type failure criterion, which is based on the hypothesis of maximum principal stress. It is assumed that material fails in tension if the maximum principal stress exceeds the uniaxial tensile stress σ_{t} and in compression, if the absolute value of minimum principal stress exceeds the uniaxial compressive strength σ_c. Such a failure surface is a cube in the principal stress space. Rankine-type cut-off approach can be used in combination to other yield/failure surfaces too, one commonly used variant is the Mohr-Coulomb criterion with tension cut-off.

Denoting the stress tensor as $\boldsymbol{\sigma}$, the Rankine-type failure surface has the form

$$f(\boldsymbol{\sigma}) = (\max(\sigma_1, \sigma_2, \sigma_3) - \sigma_\mathrm{t})(\min(\sigma_1, \sigma_2, \sigma_3) + \sigma_\mathrm{c}) = 0, \tag{23}$$

where $\sigma_i, i = 1, 2, 3$ are the principal stresses. An approximation of the Rankine type failure surface f is written as

$$f_n(\boldsymbol{\sigma}) = \mathrm{tr}(\boldsymbol{\sigma} - \alpha\mathbf{I})^n - \beta^n = 0. \tag{24}$$

If the power n is even, the parameters α and β can be solved in terms of the tensile and compressive stresses from equations

$$\alpha = \tfrac{1}{2}(\sigma_\mathrm{t} - \sigma_\mathrm{c}), \quad \beta^n = 2\left[\tfrac{1}{2}(\sigma_\mathrm{t} - \sigma_\mathrm{c})\right]^n + \left[\tfrac{1}{2}(\sigma_\mathrm{t} + \sigma_\mathrm{c})\right]^n. \tag{25}$$

The expressions of (24) in terms of the principal invariants for specific values $n = 2, 4$ and 6 are given below:

$$\begin{aligned}
f_2(I_1, I_2) &= I_1^2 + 2I_2 - 2\alpha I_1 + 3\alpha^2 - \beta^2 = 0, && (26)\\
f_4(I_1, I_2, I_3) &= I_1^4 + 4I_1^2 I_2 + 2I_2^2 - 4\alpha(I_1^3 + 3I_1I_2 + 3I_3)+ && (27)\\
&\quad + 6\alpha^2(I_1^2 + 2I_2) - 4\alpha^3 I_1 + 3\alpha^4 - \beta^4 = 0, && (28)\\
f_6(I_1, I_2, I_3) &= I_1^6 + 6I_1^4 I_2 + 6I_1^3 I_3 + 9I_1^2 I_2^2 + 12I_1I_2I_3 + 2I_2^3 + 3I_3^2+ \\
&\quad - 6\alpha(I_1^5 + 5I_1^3 I_2 + 5I_1^2 I_3 + 5I_1 I_2^2 + 5I_2I_3)+ \\
&\quad + 15\alpha^2(I_1^4 + 4I_1^2 I_2 + 4I_1I_3 + 2I_2^2)+ \\
&\quad - 20\alpha^3(I_1^3 + 3I_1I_2 + 3I_3)+ \\
&\quad + 15\alpha^4(I_1^2 + 2I_2) - 6\alpha^5 I_1 + 3\alpha^6 - \beta^6 = 0. && (29)
\end{aligned}$$

Notice that the failure surface f_2 do not depend on the third invariant I_3 which means that it is circular in the deviatoric plane. In terms of the mean and effective stress and the Lode angle θ, see (17) and (19), failure surfaces (26) and (27) take the form

$$\begin{aligned}
f_2(\sigma_\mathrm{m}, \sigma_\mathrm{e}) &= \tfrac{2}{3}\sigma_\mathrm{e}^2 + 3\sigma_\mathrm{m}^2 - 6\alpha\sigma_\mathrm{m} + 3\alpha^2 - \beta^2, && (30)\\
f_4(\sigma_\mathrm{m}, \sigma_\mathrm{e}, \cos(3\theta)) &= 3\sigma_\mathrm{m}^4 + 4\sigma_\mathrm{m}^2\sigma_\mathrm{e}^2 + \tfrac{2}{9}\sigma_\mathrm{e}^4 - 4\alpha(3\sigma_\mathrm{m}^3 + 2\sigma_\mathrm{m}\sigma_\mathrm{e}^2) + 6\alpha^2(3\sigma_\mathrm{m}^2 + \tfrac{2}{3}\sigma_\mathrm{e}^2)+ \\
&\quad - 12\alpha^3\sigma_\mathrm{m} + \tfrac{8}{9}(\sigma_\mathrm{m} - \alpha)\sigma_\mathrm{e}^3\cos(3\theta) + 3\alpha^4 - \beta^4. && (31)
\end{aligned}$$

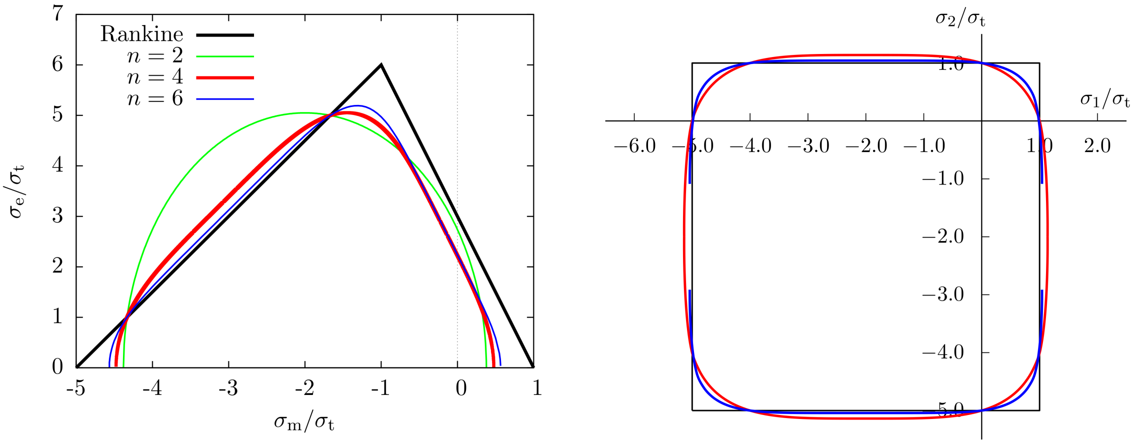
It is illustrative to show the locus of failure surface in the meridian plane, the compressive meridians of the Rankine failure surface (23) and the approximations (30) and (31) are shown in figure 2a.

The failure surface (24) has a simple appearance in the principal stress space

$$f_n(\sigma_1, \sigma_2, \sigma_3) = (\sigma_1 - \alpha)^n + (\sigma_2 - \alpha)^n + (\sigma_3 - \alpha)^n - \beta^n = 0. \tag{32}$$

In the case of plane stress, the failure surfaces have the following forms in the principal stress space:

$$\begin{aligned}
f_2 &= \sigma_1^2 + \sigma_2^2 - 2\alpha(\sigma_1 + \sigma_2) + 3\alpha^2 - \beta^2 = 0, && (33)\\
f_4 &= \sigma_1^4 + \sigma_2^4 - 4\alpha(\sigma_1^3 + \sigma_2^3) + 6\alpha^2(\sigma_1^2 + \sigma_2^2) - 4\alpha^3(\sigma_1 + \sigma_2) + 3\alpha^4 - \beta^4 = 0, && (34)\\
f_6 &= \sigma_1^6 + \sigma_2^6 - 6\alpha(\sigma_1^5 + \sigma_2^5) + 15\alpha^2(\sigma_1^4 + \sigma_2^4) - 20\alpha^3(\sigma_1^3 + \sigma_2^3)+ \\
&\quad + 15\alpha^4(\sigma_1^2 + \sigma_2^2) - 6\alpha^5(\sigma_1 + \sigma_2) + 3\alpha^6 - \beta^6 = 0. && (35)
\end{aligned}$$



(a)

(b)

Figure 2. (a) Compressive meridians for Rankine type failure criterion and approximations f_2, f_4 and f_6. (b) Plane stress case (thin black line) and its approximation as in Eq. (24) in plane stress for f_4 (thick red line) and f_6 (thick blue line). In both figures $\sigma_c = 5\sigma_t$.

In figure 2b approximations (34) and (35) are shown together with the Rankine criterion (23).

Relative errors in the corner stress value $\sigma_1 = \sigma_2 = \sigma^* > 0$ of the approximate Rankine criterion (32) are shown in figure 3. In figure 3a, the reference is the size of the failure surface, i.e. $\sigma_t + \sigma_c$, while in the 3b the reference is made wrt the tensile strength σ_t.

In computational failure analysis the direction of the damaged plane is often more important than the error in the tensile failure stress. Figure 4 shows the error in the normal direction of the approximate Rankine criterion (32) as a function of the ratio between tensile and compressive strengths for different n-values for uniaxial tensile loading. If the tensile to compressive strength ratio is of the order 0.1 (a typical value for concrete and some rocks), rather high values of the power n is required to keep the error in the fracture direction lower than e.g. 2°. A more detailed discussion and computational results are presented in a companion paper [11].

Concluding remarks

A recursion formula is given for the integer power of a second-order tensor in 3D Euclidean space. Its use is demonstrated in constitutive modelling for approximating failure or yield surfaces with corners. The Rankine failure criterion serve as an example. Use of the approximate form has the advantage that the eigenvalue problem to obtain the principal stresses need not to be solved. Errors in the corner stress values and the flow direction in the case of the associated flow rule are numerically studied.

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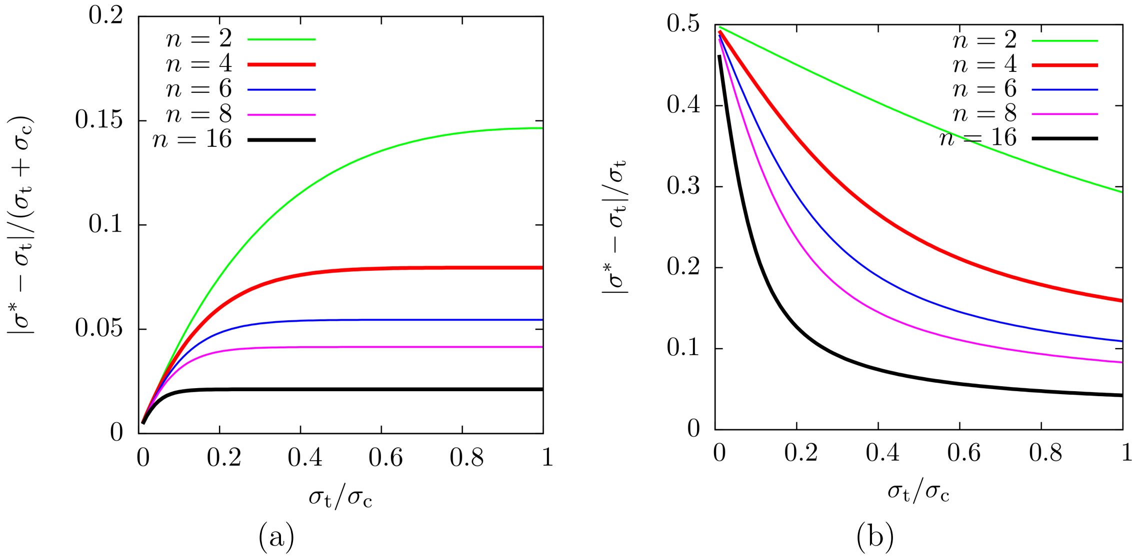

Figure 3. Relative error in the corner stress σ^* value for different values of n of the approximate Rankine criterion (32).

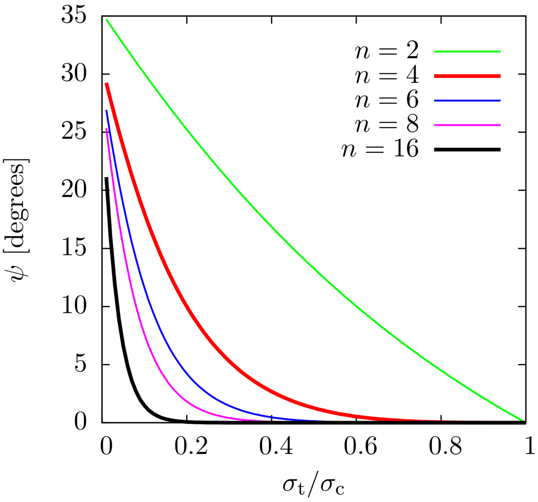

Figure 4. Error in the direction of failure surface normal in the uniaxial tensile stress case for different values of n of the approximate Rankine criterion (32).

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