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ORTHONORMAL ISOTROPIC VECTOR BASES

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ABSTRACT

Orthonormal bases of isotropic vectors for indefinite square matrices are proposed and solved. A necessary and sufficient condition is that the matrix must have zero trace. A recursive algorithm is presented for computer applications. The isotropic vectors of 3×3 matrices are solved explicitly. Deviatoric stresses in continuum mechanics, the existence of isotropic vectors (particularly in screw space), and stiffness synthesis by springs are shown to be related to the isotropic vector problem.

1 INTRODUCTION

Eigenvalue problems in mathematics, from linear algebra to differential equations, almost always have physical correspondences. They help explain complicated physical phenomena in terms that make sense to the human mind. In engineering, the concepts of principal stress, principal strain, principal axes and moments of inertia, etc. are among countless quantities that are derived from eigenvector problems with physical meanings.

In the analysis of stiffness and compliance, the eigenvalue problems provide a deeper understanding of these phenomena, especially using screw (spatial vector) algebra. The first example came from the work of Ball [2], who applied the screw theory to study rigid body motion. He investigated a generalized eigenvalue problem for stiffness, involving an indefinite metric, which lead to screws called the principal screws of the potential. Also he used the indefinite metric to determine screws of principal pitch (i.e. stationary pitch) of a subspace. The use of an indefinite quadratic form leads to the existence of isotropic vectors, i.e. vectors that make the form vanish.

In this study, bases of isotropic vectors in a space are

determined for an indefinite form. Isotropic vectors are well known, see Artin [1], Lingenberg [6]. The solution is applied to the synthesis of stiffnesses using springs in [3]. It can also be used to determine the zero and infinite pitch screws in a screw subspace. Further, the three dimensional case is explicitly solved and is physically explained using the usual stress tensor concept of continuum mechanics. The isotropic vector problem is posed as a general type of eigenvector problem.

The most significant contributions of this paper are the solution of orthonormal bases composed of isotropic vectors that span a space and a recursive algorithm for computation of the bases.

2 PRELIMINARIES

Let V be a finite dimensional vector space and $\dim(V) = n$. Let the standard Euclidean norm be defined on V such that for any $\vec{v} \in V$, $\vec{v}^T \vec{v} \geq 0$ is the square length of the vector \vec{v} . Any non-zero \vec{u} such that $\vec{u}^T \vec{u} = 1$ is called a unit vector. Any two unit vectors \vec{u}_1 and \vec{u}_2 are said to be parallel if $\vec{u}_1^T \vec{u}_2 = 1$ and orthogonal (or perpendicular, reciprocal, etc.) if $\vec{u}_1^T \vec{u}_2 = 0$.

The action of an $n \times n$ square matrix A (a linear operator) on a vector, $A\vec{u}$, is composed of two parts: 1) a rotation and 2) a scaling. Rotation is understood in the sense of length invariance. For example, orthogonal matrices defined by $UU^T = I$ only perform rotations.

An eigenvalue problem on V is given as

$$A\vec{u} = \lambda\vec{u} \quad (1)$$

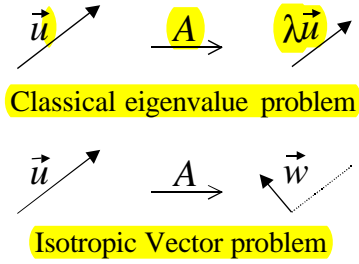


Figure 1. Comparison of the eigenvector and isotropic vector problems.

where $\vec{u} \in V$, A is a square matrix, and λ is a scalar. The eigenvalue problem (1) is about the existence of a vector \vec{u} which is transformed into a parallel vector $\lambda\vec{u}$. In other words, \vec{u} is scaled by A , but not rotated. Such vectors \vec{u} and scalars λ are the eigenvectors and eigenvalues of A . It is well known that the eigenvectors, with the constraint $\vec{u}^T \vec{u} = 1$, make the quadratic form $\vec{u}^T A \vec{u}$ stationary. For a more detailed analysis of eigenvector problem and associated matrix methods see, for example, Horn and Johnson [5], Pease [7].

In the proposed isotropic vector problem, a non zero vector is scaled and rotated to an orthogonal direction. Figure 1 illustrates the eigenvector and isotropic vector problems geometrically.

3 THE ISOTROPIC VECTOR PROBLEM

Definition 1. For a square matrix A , any vector \vec{u} satisfying

$$A\vec{u} = \vec{w} \quad \vec{u}^T \vec{w} = 0 \quad (2)$$

is called an **isotropic vector** of A .

The following lemmas follow directly from (2).

Lemma 2. A vector \vec{u} is an isotropic vector of A if and only if $\vec{u}^T A \vec{u} = 0$.

Considering the quadratic form induced by A as a scalar valued vector function, the eigenvectors are the stationary points and the isotropic vectors are the zero locus.

Lemma 3. The isotropic vectors of a matrix A are identical to those of its symmetric part.

Proof. This follows from $\vec{u}^T A \vec{u} = \vec{u}^T A_{\text{sym}} \vec{u} + \vec{u}^T A_{\text{skew}} \vec{u} = \vec{u}^T A_{\text{sym}} \vec{u}$. \diamond

This is an interesting difference between the eigenvector and the isotropic vector problems, indicating that it is sufficient to restrict the analysis to symmetric matrices only. So, unless otherwise is noted, A is assumed to be symmetric throughout.

4 EXISTENCE OF ISOTROPIC VECTORS

For any matrix A , if $\vec{v} \in \mathcal{N}(A)$, where $\mathcal{N}(A)$ is the null space of A , then $A\vec{v} = \vec{0}$ by definition, thus $\vec{v}^T A \vec{v} = 0$. So, any vector in $\mathcal{N}(A)$ is an isotropic vector. Such isotropic vectors are considered trivial. The following theorem gives the condition for the existence of non trivial isotropic vectors.

Theorem 4. A has non trivial isotropic vectors if and only if it is indefinite.

Proof. Let \vec{v} be a non trivial isotropic vector. Then, $\vec{v}^T A \vec{v} = 0$, $\vec{v} \notin \mathcal{N}(A)$ and, by definition, A is indefinite. Conversely, let A be an indefinite matrix with eigenvalues λ_i ($i = 1, \dots, n$) such that $\lambda_1 = \max(\lambda_i) > 0$ and $\lambda_n = \min(\lambda_i) < 0$. Consider a vector \vec{v} as a point of \mathcal{R}^n . Then, the quadratic form $\vec{v}^T A \vec{v}$ is a continuous function from \mathcal{R}^n into \mathcal{R} . It is well known that $\vec{v}_1^T A \vec{v}_1 > 0 > \vec{v}_n^T A \vec{v}_n$, where \vec{v}_1 and \vec{v}_n are the eigenvectors corresponding to λ_1 and λ_n . Consider any smooth curve $\vec{\xi}(t)$ from \vec{v}_1 to \vec{v}_n parametrized by t . Then, $\vec{v}^T A \vec{v}(t)$ is a continuous function of t along the curve. So, by mean value theorem, $\vec{v}^T A \vec{v}(t)$ takes on every value in $[\vec{v}_n^T A \vec{v}_n, \vec{v}_1^T A \vec{v}_1]$. Hence, there exists a t_0 such that $\vec{v}^T A \vec{v}(t_0) = 0 \in [\vec{v}_n^T A \vec{v}_n, \vec{v}_1^T A \vec{v}_1]$. In particular, for all smooth curves restricted to the plane formed by \vec{v}_1 and \vec{v}_n , the points on the curve represents vectors which are simply the linear combinations of \vec{v}_1 and \vec{v}_n and, therefore, not in the null space of A . Then, the points at which the quadratic form vanish give the non trivial isotropic vectors. \diamond

Let \vec{v}_1 and \vec{v}_2 be such that $\vec{v}_1^T A \vec{v}_1 > 0 > \vec{v}_2^T A \vec{v}_2$ and consider all vectors in the plane formed by \vec{v}_1 and \vec{v}_2 . These can be given as $\vec{v} = a_1 \vec{v}_1 + a_2 \vec{v}_2$. This plane contains the origin and the quadratic form changes sign on it. Since \vec{v}_1 and \vec{v}_2 are not solutions to $\vec{v}^T A \vec{v} = 0$ one can take $a_i \neq 0$. Also, the magnitude of \vec{v} is insignificant. Therefore, the direction of \vec{v} is completely characterized by $\vec{v} = \vec{v}_1 + a \vec{v}_2$. Now, the quadratic equation becomes

$$\vec{v}^T A \vec{v} = \vec{v}_2^T A \vec{v}_2 a^2 + 2\vec{v}_1^T A \vec{v}_2 a + \vec{v}_1^T A \vec{v}_1 = 0 \quad (3)$$

The discriminant of this equation is always positive since $(\vec{v}_2^T A \vec{v}_2)(\vec{v}_1^T A \vec{v}_1) < 0$. As a result there exist two distinct real solutions for a . Hence the following is proven.

Theorem 5. *If the quadratic form $\vec{v}^T A \vec{v}$ changes sign on a plane containing the origin then there exist two distinct lines on which it vanishes. The directions of these lines give two distinct isotropic vectors.*

Corollary 6. *For an indefinite matrix A , there exist infinitely many distinct isotropic vectors if $n > 2$, and there exist exactly two isotropic vectors if $n = 2$.*

Proof. For $n = 1$, A cannot be indefinite. Therefore, $n \geq 2$.

For $n = 2$, there exists only one plane through the origin. The quadratic form changes sign on this plane since there are two lines on which it has opposite signs due to indefiniteness. Then, by Theorem 5, there exists two isotropic vectors.

For $n > 2$, there exist infinitely many planes through the origin. Since A is indefinite, the quadratic form changes sign on at least one plane, say π , spanned by two vectors \vec{v}_1 and \vec{v}_2 . Let the quadratic form be positive for \vec{v}_1 and negative for \vec{v}_2 . Since $n > 2$, there exist vectors \vec{v}'_2 which are not in π . By continuity, there exists a \vec{v}'_2 sufficiently close to \vec{v}_2 , such that the quadratic form is still negative at \vec{v}'_2 . Thus, \vec{v}_1 and \vec{v}'_2 span a plane π' containing the origin, on which the quadratic form changes sign. In this way, one obtains infinitely many such planes. So, by Theorem 5, there exist infinitely many isotropic vectors for $n > 2$. \diamond

From Corollary 6, every indefinite matrix of order n has at least n isotropic vectors. So, let $U = [\vec{u}_1, \dots, \vec{u}_n]$ be a square matrix formed from any n isotropic vectors, and $W = [\vec{w}_1, \dots, \vec{w}_n]$ be the corresponding vectors, $\vec{u}_i^T \vec{w}_i = 0$. Then, by definition, $AU = W$. Premultiplying both sides by U^T one gets

$$U^T AU = U^T W = \begin{bmatrix} \vec{u}_1^T \\ \vdots \\ \vec{u}_n^T \end{bmatrix} [\vec{w}_1, \dots, \vec{w}_n] \quad (4)$$

$$= \begin{bmatrix} \vec{u}_1^T \vec{w}_1 & \dots & \vec{u}_1^T \vec{w}_n \\ \vdots & \ddots & \vdots \\ \vec{u}_n^T \vec{w}_1 & \dots & \vec{u}_n^T \vec{w}_n \end{bmatrix} \quad (5)$$

But, the diagonal elements are $\vec{u}_i^T \vec{w}_i = 0$. Hence, the following theorem is proven.

Theorem 7. *Every indefinite matrix is congruent to a matrix whose diagonal elements are all zero.*

A particular solution which is used in the next section is the following.

Theorem 8. *If $\lambda_1 > 0$ and $\lambda_2 < 0$ are any two eigenvalues, and, \vec{v}_1 and \vec{v}_2 are any two corresponding eigenvectors of a symmetric A , then two isotropic vectors are given by*

$$\vec{u}_{1,2} = \sqrt{-\lambda_2} \vec{v}_1 \pm \sqrt{\lambda_1} \vec{v}_2 \quad (6)$$

Proof. One only needs to use the well known properties of eigenvectors of symmetric matrices, namely, $\vec{v}_i^T A \vec{v}_j = \delta_{ij} \lambda_i$. Then

$$\begin{aligned} \vec{u}_i^T A \vec{u}_i &= \left(\sqrt{-\lambda_2} \vec{v}_1 \pm \sqrt{\lambda_1} \vec{v}_2 \right)^T A \left(\sqrt{-\lambda_2} \vec{v}_1 \pm \sqrt{\lambda_1} \vec{v}_2 \right) \\ &= -\lambda_2 \vec{v}_1^T A \vec{v}_1 + \lambda_1 \vec{v}_2^T A \vec{v}_2 \\ &= -\lambda_2 \lambda_1 + \lambda_1 \lambda_2 = 0 \quad \diamond \end{aligned} \quad (7)$$

Corollary 9. *The isotropic vectors of Theorem 8 are orthogonal ($\vec{u}_1^T \vec{u}_2 = 0$) if and only if $\lambda_1 = -\lambda_2$.*

Proof. By Theorem 8,

$$\begin{aligned} \vec{u}_1^T \vec{u}_2 &= \left(\sqrt{-\lambda_2} \vec{v}_1 + \sqrt{\lambda_1} \vec{v}_2 \right)^T \left(\sqrt{-\lambda_2} \vec{v}_1 - \sqrt{\lambda_1} \vec{v}_2 \right) \\ &= -(\lambda_2 + \lambda_1) \end{aligned} \quad (8)$$

from which the corollary follows. \diamond

The following theorem shows that there always exists a complete basis of isotropic vectors for every indefinite matrix.

Theorem 10. *There exists n linearly independent isotropic vectors for any indefinite matrix A of order n .*

Proof. Any vector in the null space of A is an isotropic vector. So, if $r = \text{rank}(A)$ then there always exist $n - r$ isotropic vectors spanning the null space. Therefore, it is sufficient to prove the theorem for the r dimensional subspace spanned by the eigenvectors belonging to non-zero eigenvalues. Proof is obtained by induction. Let λ_i and \vec{v}_i be the eigenvalues and eigenvectors. Among the r eigenvalues there exists at least one pair of eigenvalues with opposite signs due to the indefiniteness. So, there always exists at least $q \leq r$ eigenvalues with mixed signs.

1. Assume that there exists a q dimensional subspace spanned by q eigenvectors $\{\vec{v}_i, i = 1, \dots, q\}$ corresponding to eigenvalues with mixed signs, which is also spanned by q isotropic vectors $\{\vec{u}_i, i = 1, \dots, q\}$.

2. Then, consider any of the remaining $r - q$ eigenvectors, say \vec{v}_{q+1} . Regardless of the sign of λ_{q+1} , there exists an eigenvalue with an opposite sign in the original set of q eigenvalues, say λ_1 . Then, by Theorem 8, the plane spanned by \vec{v}_1 and \vec{v}_{q+1} contains two distinct isotropic vectors which are not in the space spanned by $\{\vec{v}_i, i = 1, \dots, q\}$, or $\{\vec{u}_i, i = 1, \dots, q\}$. Therefore, using either of these isotropic vectors, say \vec{u}_{q+1} , one obtains a linearly independent set $\{\vec{u}_i, i = 1, \dots, q + 1\}$ of $q + 1$ isotropic vectors which span the subspace spanned by $\{\vec{v}_i, i = 1, \dots, q + 1\}$.
3. Finally, since the assumption is valid for $q = 2$, Theorem 8, it is valid for any q .

The theorem is completed by also adding any $n - r$ linearly independent null space vectors.◊

5 ORTHONORMAL SETS OF ISOTROPIC VECTORS

As an analogy with the eigenvalue problem, one may ask whether there can be n mutually orthogonal isotropic vectors of a matrix. Assume there exists such a set of isotropic vectors. Let $U = [\vec{u}_i]$ be an orthogonal matrix formed from these n elements. Then, by Theorem 7, $\Phi = U^T A U$ is a matrix with zero diagonal, and therefore zero trace. However, since U is orthogonal, $U^T U = I$. Therefore,

$$0 = \text{trace}(\Phi) = \text{trace}(U^T A U) \quad (9)$$

$$= \text{trace}(U^T U A) = \text{trace}(A) \quad (10)$$

This gives the following necessary condition.

Theorem 11. *If a matrix A of order n has an orthogonal set of n isotropic vectors then $\text{trace}(A) = 0$.*

Note that, if a matrix has n mutually orthogonal isotropic vectors then $U^T A U$ is an orthogonal transformation of A . In a basis formed by these vectors, A has zero diagonals. This result is complementary to case of the eigenvector problem where a symmetric matrix becomes diagonal when expressed in an orthogonal basis comprised of its eigenvectors.

Corollary 6 that was stated for indefinite matrices applies to zero traces matrices after a slight modification.

Corollary 12. *A matrix A , such that $\text{trace}(A) = 0$, has infinitely many distinct isotropic vectors if $n > 2$, or, $n = 2$ and $A = 0$. It has exactly one and two isotropic vectors for $n = 1$ and $n = 2$ ($A \neq 0$), respectively.*

Proof. A zero trace matrix A is either zero or indefinite. If $n = 1$ then $A = 0$ and there exists a unique isotropic vector.

If $n > 1$ and $A = 0$ then there exist infinitely many distinct isotropic vectors. If A is indefinite then Corollary 6 applies. This proves the corollary.◊

It is desired to determine if a zero trace matrix A can have a complete orthogonal set of isotropic vectors. This is investigated below by using the separate cases identified in Corollary 12.

For $A = 0$, any orthonormal set of n vectors is an orthonormal set of isotropic vectors. So, $A = 0$ cases are trivial for all n .

For $n = 1$, $A = 0$. Therefore, the solution is trivial.

For $n = 2$ and $A \neq 0$, there exists only two distinct isotropic vectors, Corollary 12. However, $\text{trace}(A) = \lambda_1 + \lambda_2 = 0$ and the isotropic vectors are orthogonal by Corollary 9.

Only the cases with $n > 2$ ($A \neq 0$) are left to consider. By Corollary 12, there exist infinitely many isotropic vectors in this case. Given an indefinite matrix, one can always find an isotropic vector by using Theorem 8. The question is to find another that is orthogonal to the first when $n > 2$. If a suitable method is developed to do this, then it can be repeatedly applied to find a series of orthogonal isotropic vectors. The process should stop naturally when n such vectors are obtained. The following discussion and theorems present a recursive algorithm that generates an orthonormal set of isotropic vectors.

For eigenvalue problems, there exists a method that sequentially and recursively generates the eigenvalues and corresponding eigenvectors. Let A be a symmetric matrix. A can be assumed to be positive definite. If it is not, one can always perform a shifting of the eigenvalues by $A' = A + kI$, where $k > |\min(\lambda_i)|$. The matrices A and A' have the same eigenvectors. Their eigenvalues are related by $\lambda'_i = \lambda_i + k$, so that A' is positive definite. Let the eigenvalues be ordered such that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.

Many numerical procedures, if used without modification, usually fail to find all eigenvalues, even if they are used with different initial guesses. A method used to overcome this difficulty is based on the fact that, for any symmetric positive definite matrix A , the matrix $A - \lambda_i \vec{v}_i \vec{v}_i^T$, where λ_i is any eigenvalue with the corresponding eigenvector \vec{v}_i , retains all the eigenvalues of A except λ_i which is replaced by zero. The eigenvectors are all identical. This is sometimes called *deflating* a matrix. So, if λ_n and \vec{v}_n is found by any means, then one constructs $A_2 = A - \lambda_n \vec{v}_n \vec{v}_n^T$. Then, one performs an orthogonal transformation such that \vec{v}_n is one of the standard basis vectors. In this system, $A_2 = \begin{bmatrix} 0 & \vec{0}^T \\ \vec{0} & A_2^* \end{bmatrix}$, where A_2^* is an $(n - 1) \times (n - 1)$ matrix whose eigenvalues are $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1}$. So, by applying a numerical procedure, one finds λ_{n-1} and \vec{v}_{n-1}^* . Repeating the procedure

in this way, one determines all eigenvalues and eigenvectors. It is this method that inspires the following theorem.

Theorem 13. *If \vec{u} is a unit isotropic vector of A , $\text{trace}(A) = 0$, $A\vec{u} = \vec{w}$, then there exists a symmetric matrix A^* given by*

$$A^* = A - \vec{w}\vec{u}^T - \vec{u}\vec{w}^T \quad (11)$$

such that

1. $\text{trace}(A^*) = 0$
2. \vec{u} is in the null space of A^* .
3. For $n > 1$, A and A^* have common isotropic vectors orthogonal to \vec{u} . For $n = 1$, $A = A^* = 0$.

Proof. (1) For any two vectors \vec{a} and \vec{b} , $\text{trace}(\vec{a}\vec{b}^T) = \vec{a}^T\vec{b}$. Then, by using $\text{trace}(A) = 0$ and $\vec{w}^T\vec{u} = 0$ in (11),

$$\begin{aligned} \text{trace}(A^*) &= \text{trace}(A) - \text{trace}(\vec{w}\vec{u}^T + \vec{u}\vec{w}^T) \\ &= 0 - \vec{u}^T\vec{w} - \vec{w}^T\vec{u} = 0 \end{aligned} \quad (12)$$

(2) Next, by multiplying (11) by \vec{u} , and, using $\vec{u}^T\vec{u} = 1$ and $\vec{w}^T\vec{u} = 0$, one gets

$$A^*\vec{u} = [A - \vec{w}\vec{u}^T - \vec{u}\vec{w}^T]\vec{u} = A\vec{u} - \vec{w} = \vec{0} \quad (13)$$

(3) Finally, if \vec{u}' is orthogonal to \vec{u} then, from (11), $\vec{u}'^T A^* \vec{u}' = \vec{u}'^T A \vec{u}'$. So, the quadratic forms of A and A^* have identical values in the subspace orthogonal to \vec{u} . Therefore, if \vec{u}' is an isotropic vector of A^* orthogonal to \vec{u} then it is also an isotropic vector of A , and vice versa. \diamond

Corollary 14. *For any zero trace symmetric matrix A , there exists a finite sequence of zero trace symmetric matrices, $A = A_1, A_2, \dots, A_n = 0$, recursively given by*

$$A_{i+1} = A_i - \vec{u}_i \vec{w}_i^T - \vec{w}_i \vec{u}_i^T \quad (14)$$

where \vec{u}_i is an isotropic vector of A_i , $A_i \vec{u}_i = \vec{w}_i$, such that

1. $A_i \vec{u}_j = \vec{0}$, for all $j < i$.
2. $\{\vec{u}_i\}$ is an orthonormal set.
3. \vec{u}_i is an isotropic vector of all A_j , $j \leq i$.

Proof. If $n = 1$ then $A_1 = 0$ and the sequence is determined. Statements of the theorem are trivially true. If $n = 2$, then the two orthogonal isotropic vectors of A_1 are given by Corollary 9. Then, A_2 has zero trace and a zero eigenvalue, that is $A_2 = 0$ which ends the sequence.

So, assume $n > 2$. A proof by induction is used. Assume that (1), (2) and (3) are true for some i . Then,

1. for $j < i + 1$

$$\begin{aligned} A_{i+1} \vec{u}_j &= A_i \vec{u}_j - \vec{u}_i \vec{w}_i^T \vec{u}_j - \vec{w}_i \vec{u}_i^T \vec{u}_j \\ &= \begin{cases} A_i \vec{u}_i - \vec{w}_i = \vec{0} & j = i \\ -\vec{u}_i \vec{w}_i^T \vec{u}_j = -\vec{u}_i \vec{u}_i^T (A_i \vec{u}_j) = \vec{0} & j < i \end{cases} \end{aligned} \quad (15)$$

which proves that $A_{i+1} \vec{u}_j = \vec{0}$ for all $j < i + 1$. This means that all \vec{u}_j , $j < i + 1$, are in the null space of A_{i+1} .

2. By Theorem 13, an isotropic vector of A_{i+1} , \vec{u}_{i+1} , exists which is not in the subspace spanned by $\{\vec{u}_i\}$. So, $\{\vec{u}_i\}, \vec{u}_{i+1}$ is an orthogonal set.
3. Finally, by applying Theorem 13 again, one concludes that \vec{u}_{i+1} is an isotropic vector of A_j for all $j \leq i + 1$. \diamond

This corollary proves that the zero trace condition is sufficient for a symmetric matrix to have n orthonormal isotropic vectors. Combining with Theorem 11, the following main result of this section yields,

Corollary 15. *A matrix A of order n has a complete orthonormal set of n isotropic vectors if and only if $\text{trace}(A) = 0$.*

Corollary 16. *Any matrix A of order n is orthogonally congruent to a matrix with identical diagonal elements.*

Proof. For any A , $A' = A - \frac{1}{n} \text{trace}(A) I$ is a zero trace matrix. By Corollary 15, A' is orthogonally congruent to a matrix Φ with zero diagonals, i.e. $U^T A' U = \Phi$, $U^T U = I$. Therefore,

$$U^T A U = U^T A' U + \frac{1}{n} \text{trace}(A) U^T U \quad (16)$$

$$= \Phi + \frac{1}{n} \text{trace}(A) I \quad (17)$$

which is a matrix with all diagonal entries equal to $\frac{1}{n} \text{trace}(A)$. \diamond

Corollary 14 provides a recursive method for the construction of an orthonormal set of n isotropic vectors of arbitrary zero trace matrices. The following is a working algorithm that utilizes Theorem 8.

1. Read $n \times n$ matrix M
2. If $\text{trace}(M) \neq 0$ Stop. No solution
3. Symmetric part: $A = \frac{1}{2}(M + M^T)$
4. Initialize: $U = \mathcal{N}(A)$
5. Loop: while $A \neq 0$,
6. λ_i = eigenvalues, \vec{v}_i = eigenvectors of A
7. $\lambda_p = \max(\lambda_i)$, $\lambda_m = \min(\lambda_i)$
8. $\vec{u} = \text{Normalize}[\sqrt{-\lambda_m} \vec{v}_p + \sqrt{\lambda_p} \vec{v}_m]$

9. Concatenate $U = [U : \vec{u}]$
10. $\vec{w} = A\vec{u}$
11. $A = A - \vec{w}\vec{u}^T - \vec{u}\vec{w}^T$
12. If $-\lambda_m = \lambda_p$ Then,
13. $\vec{u} = \text{Normalize} [\sqrt{-\lambda_m}\vec{v}_p - \sqrt{\lambda_p}\vec{v}_m]$
14. Concatenate $U = [U : \vec{u}]$
15. $\vec{w} = A\vec{u}$
16. $A = A - \vec{w}\vec{u}^T - \vec{u}\vec{w}^T$
17. End If
18. $A = \frac{1}{2}(A + A^T)$
19. End Loop

The above algorithm has been tested numerically, using MATLAB, and yielded good results. The second statement from the bottom seems to be necessary for numerical stability. Note that whenever $\min(\lambda_i) = -\max(\lambda_i)$, both isotropic vectors predicted by Theorem 8 are used since they are already orthogonal in that case, Corollary 9. But, the actual reason is different. In general, the recursion in Corollary 14 gives $\text{rank}(A_{i+1}) = \text{rank}(A_i) - 1$. However, for any two eigenvalues with equal magnitudes and opposite signs, any of the isotropic vectors of Theorem 8 makes $\text{rank}(A - \vec{w}_1\vec{u}_1^T - \vec{u}_1\vec{w}_1^T) = \text{rank}(A) - 2$. Proof of this fact is not difficult, but omitted here. Then, one can also show that the other vector predicted by Theorem 8, $\vec{u}_2 \perp \vec{u}_1$, is also in the null space of the new matrix. Since the algorithm is basically a recursion based on the column spaces of current matrices, \vec{u}_2 must be added to the set or, otherwise, the algorithm returns a deficient set.

5.1 Multitude of Solutions

It was shown earlier that a trace zero matrix has infinitely many isotropic vectors if $n > 2$, or, $n = 2$ and $A = 0$. So, a natural question is about the multitude of solutions to the orthonormal set problem. Note that if there exists such a set then,

$$U^T A U = \Phi = \begin{bmatrix} 0 & \bullet & \bullet \\ \bullet & \ddots & \bullet \\ \bullet & \bullet & 0 \end{bmatrix} \quad (18)$$

An $n \times n$ orthogonal matrix has $\frac{1}{2}n(n-1)$ independent parameters. Since only the diagonals are to be satisfied, the above matrix equation is equivalent to n scalar quadratic equations in terms of the parameters of U . However, due to the trace condition one of these equations is dependent on others, leaving $(n-1)$ equations in $\frac{1}{2}n(n-1)$ parameters. This gives a net of $\frac{1}{2}n(n-1) - (n-1) = \frac{1}{2}(n-1)(n-2)$ free parameters in general. For $n = 1, 2$ this gives 0 free parameters, meaning finitely many solutions as shown

earlier ($n = 2$, $A = 0$ is a degenerate case). For $n = 3$ there is $\frac{1}{2}(3-1)(3-2) = 1$ free parameter. This is demonstrated in the next section.

5.2 Closed Form Solutions for 3D

In this section, the orthogonal sets of isotropic vectors of 3×3 matrices are found explicitly, i.e. without using the recursive algorithm presented earlier. To do this, one uses the well known fact that for orthogonal transformations such as $U^T A U = \Phi$, A and Φ must have the same characteristic equation. In three dimensions, the characteristic equation is

$$\det(A - \lambda I) = \det(\Phi - \lambda I) = \lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 = 0 \quad (19)$$

whose solutions λ_i are the eigenvalues of A and Φ . The coefficients I_i are called the **invariants**. By expressing A in diagonal form, which does not affect the invariants, one shows that

$$I_1 = \lambda_1 + \lambda_2 + \lambda_3 = \text{trace}(A) = 0 \quad (20)$$

$$I_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \quad (21)$$

$$I_3 = \lambda_1\lambda_2\lambda_3 = \det(A) \quad (22)$$

But, the form of Φ is already known to be

$$\Phi = \begin{bmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{bmatrix} \quad (23)$$

which gives the invariants as

$$I_1 = 0 \quad (24)$$

$$I_2 = -(a^2 + b^2 + c^2) \quad (25)$$

$$I_3 = 2abc \quad (26)$$

Given A , I_i can be calculated. Therefore, any solution Φ must satisfy (25) and (26) in terms of unknowns a, b, c .

In abc coordinates, (25) represents a *sphere*. Since $I_1 = 0$, one easily shows by $I_1^2 = 0$ that $I_2 \leq 0$ which is necessary and sufficient condition for the sphere to have real points. For $I_2 = 0$ and real a, b, c , the solution is trivial since $a = b = c = 0$, and both matrices must vanish. So, assume $I_2 < 0$. With this assumption, A can have at most one zero eigenvalue. Let λ_i be ordered so that $\lambda_1 \geq \lambda_2 \geq \lambda_3$.

Equation (26), on the other hand, is a *third order surface* that has four disconnected components if $I_3 \neq 0$. This

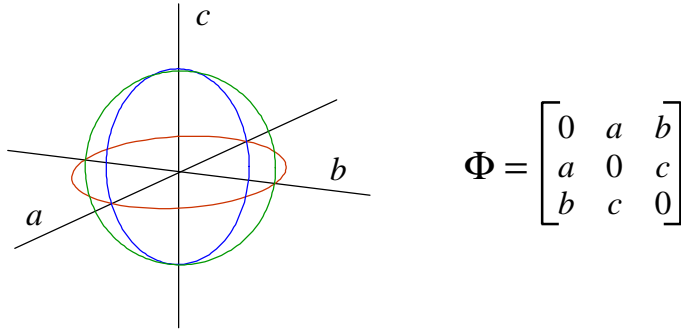


Figure 2. Solutions to the isotropic vector problem in 3-dimensions for the degenerate case: $\det(A) = 0$. The three circles are of the same radius and centered at the origin of abc -space. Each circle is in a distinct coordinate plane.

is because if $\{a_0, b_0, c_0\}$ is a point on the third order surface then so is any triplet obtained by reversing the signs of any two entries, such as $\{-a_0, -b_0, c_0\}$, giving a total of four points, each located in a distinct octant. These components are disconnected since it is not possible to trace any connected curve from $\{a_0, b_0, c_0\}$ to, say, $\{-a_0, -b_0, c_0\}$ without making $I_3 \neq 0$.

The intersection of the sphere and the third order surface is the solution set. Also, note that if $\{a_0, b_0, c_0\}$ is a solution, so is any permutation of it.

If there exists a zero eigenvalue it must be λ_2 due to ordering. In this case $I_3 = 0$. Then at least one of a, b, c is zero. Let $c = 0$. The others are obtained by permutations. Then, (26) is identically satisfied, and (25) reduces to $a^2 + b^2 = -I_2$. This is a circle. So, all solutions $\{a, b, c\}$ are given by $\sqrt{-I_2}\{\cos \theta, \sin \theta, 0\}$, where θ is arbitrary. Sign reversals give the same circle and permutations give circles in different planes. A total of three circles exist. Figure 2 illustrates these circles.

Now, assume $I_3 \neq 0$. Treating $c \neq 0$ as a parameter one gets two equations in a and b as

$$a^2 + b^2 = -I_2 - c^2 \quad (27)$$

$$2ab = I_3/c \quad (28)$$

By adding and subtracting these two equations from each other one gets

$$(a + b)^2 = I_3/c - I_2 - c^2 = \alpha(c) \quad (29)$$

$$(a - b)^2 = -I_3/c - I_2 - c^2 = \beta(c) \quad (30)$$

For real solutions $\alpha, \beta \geq 0$. There are two solutions;

$$a = \frac{\pm\sqrt{\alpha} \pm \sqrt{\beta}}{2} \quad (31)$$

$$b = \frac{\pm\sqrt{\alpha} \mp \sqrt{\beta}}{2} \quad (32)$$

which are real if and only if $\alpha, \beta \geq 0$ (either upper or lower signs are to be used for both a and b). For any given c these indicate two points in two distinct components. It is left to determine if there exist values of c for which $\alpha, \beta \geq 0$.

The conditions $\alpha, \beta \geq 0$ can be multiplied by c to give

$$c\alpha, c\beta \geq 0 \quad \text{for} \quad c > 0 \quad (33)$$

$$c\alpha, c\beta \leq 0 \quad \text{for} \quad c < 0 \quad (34)$$

Define functions $f^- = c^3 + I_2c - I_3$ and $f^+ = c^3 + I_2c + I_3$. Then, by using (29) and (30), and reversing signs, give

$$f^\mp = c^3 + I_2c \mp I_3 \begin{cases} \leq 0 & \text{for } c > 0 \\ \geq 0 & \text{for } c < 0 \end{cases} \quad (35)$$

That is, the functions f^+ and f^- must be both negative for positive c and both positive for negative c . Let $f^0 = c^3 + I_2c$. Then, f^+ and f^- are obtained by adding and subtracting the same constant, which amounts to vertical shifts of their graphs. Also, note that f^- is simply the characteristic polynomial. Therefore, it always has three real roots. It is also not difficult to show that if λ_i is a root of f^- , then $-\lambda_i$ is a root of f^+ . Therefore, f^+ has three real roots, too. This is illustrated in Figure 3 for $I_3 > 0$. The solution set is denoted by thick line segments. $I_3 < 0$ case is similar.

The solution regions for c are

$$c \in \begin{cases} [\lambda_3, \lambda_2] \cup [-\lambda_2, -\lambda_3] & \text{for } I_3 > 0 \\ [-\lambda_1, -\lambda_2] \cup [\lambda_2, \lambda_1] & \text{for } I_3 < 0 \end{cases} \quad (36)$$

which has two disconnected regions in any case. Together with the solutions of a and b , the total real solution space is composed of four distinct components which are described by one free parameter c , as claimed in the previous section.

Any solution (a, b, c) means at least one 3×3 rotation matrix U such that $U^T A U = \Phi$. The columns of U give a set of three orthonormal isotropic vectors of A .

Degenerate cases exist for double eigenvalues which reduces the solutions for Φ to a finite number of isolated

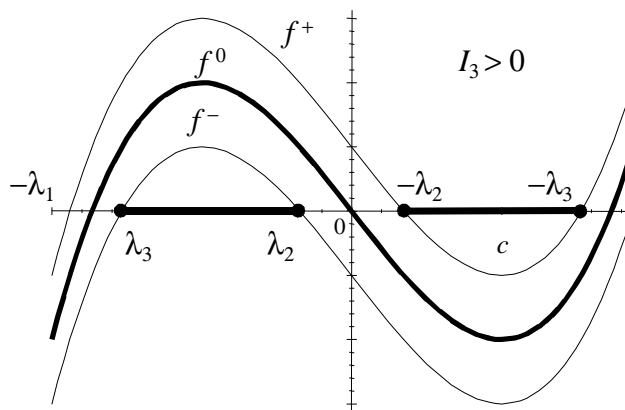


Figure 3. Solution regions for the parameter c . General case.

points, namely

$$\left[\begin{array}{l} \text{if } \lambda_3 = \lambda_2 \text{ and } I_3 > 0 \text{ or} \\ \text{if } \lambda_1 = \lambda_2 \text{ and } I_3 < 0 \end{array} \right] \text{ then } c \in \{\pm\lambda_2\} \quad (37)$$

In degenerate cases, a single point (a, b, c) corresponds to infinitely many U . This is due to the existence of a double eigenvalue. In other words, if U is a solution corresponding to (a, b, c) , then all RU are solutions, where R is a rotation matrix about the axis corresponding to the single eigenvalue, which essentially keeps the matrices unchanged. This defines a 1-parameter family for U . As a result, although in the degenerate case the solutions (a, b, c) are isolated points, the space of corresponding U is still a 1-parameter family.

To see how U can be obtained from knowledge of A and Φ , let R_A be the rotation matrix formed by the eigenvectors of A and R_Φ be that for Φ . Since both A and Φ have the same eigenvalues then

$$R_A^T A R_A = R_\Phi^T \Phi R_\Phi = \text{diag}[\lambda_1 \ \lambda_2 \ \lambda_3] \quad (38)$$

Note that the eigenvalues must be ordered in the same way when determining R_A and R_Φ . Then,

$$(R_\Phi R_A^T) A (R_A R_\Phi^T) = \Phi \quad (39)$$

from which one concludes

$$U = R_A R_\Phi^T \quad (40)$$

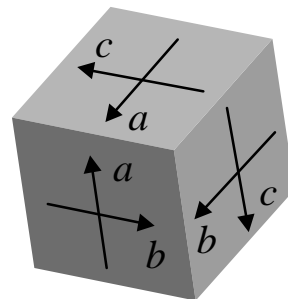


Figure 4. A stress element with pure shear stresses. The normals of the surfaces correspond to an orthonormal set of special eigenvectors. Shear values are given by a, b, c which make up the matrix Φ .

Note again that if there is a double eigenvalue in λ_i , both R_A and R_Φ are non-unique and commonly defined by one parameter.

6 EXAMPLES

6.1 Continuum Mechanics

The 3-dimensional problem has a physical explanation in the context of continuum mechanics. The stress tensor is taken as an example. However, the results trivially extend to strain tensor.

It is well known in continuum mechanics that the stress tensor at any point of a material is given by a 3×3 symmetric matrix. Any stress tensor σ can be decomposed into its hydrostatic ($\frac{1}{3}\text{trace}(\sigma)\mathbf{I}$), and deviatoric (σ') components. This is identical to what is essentially done in Corollary 16. The hydrostatic component is a pure normal stress state of equal magnitude in every direction. σ' is considered to correspond to pure shear loading. This is sensible since, by the fact that $\text{trace}(\sigma') = 0$, there exists a coordinate system in which σ' has zero diagonals (i.e. no normal stresses) by Corollary 16. Figure 4 illustrates such a state which is a pure shear state. By the results of the previous and current sections, these coordinates correspond to the isotropic vectors of σ' and, in general, there exists infinitely many of them described by one parameter. This is illustrated in Figure 5 which shows the Mohr's circle representation of three dimensional deviatoric stress. All possible stress states are in the shaded region. The thick lines correspond to distinct pure shear states which is in agreement with what is claimed here, a one parameter family. If two principal stresses are equal then one circle degenerates to a point and the other two coincide, giving only two such pure shear states as claimed.

6.2 Screw Theory and Isotropic Vectors

The space of screws, or spatial vectors, is a 6-dimensional vector space on which there exists a transformation given by the group of rigid body motions. A screw can be represented as a 6×1 vector $\hat{S} = [\vec{a}^T, \vec{b}^T]^T$, where \vec{a} and \vec{b} are 3-vectors. When \vec{a} is a translation and \vec{b} is a rotation, the screw is called a *twist*. When \vec{a} is a force and \vec{b} is a moment, it is called a *wrench*. In this way, the twists are represented in axis-coordinates and wrenches are represented in ray-coordinates, demonstrating the geometric duality. For a screw in ray-coordinates, the rigid body transformation applies as $[(\mathbf{R}\vec{a})^T, (\mathbf{R}\vec{b} + \mathbf{R}(\vec{a} \times \vec{r}))^T]^T$, where \mathbf{R} is a rotation and \vec{r} is a translation. The pitch of a screw in ray-coordinates is the scalar $h = \frac{\vec{a}^T \vec{b}}{\vec{a}^T \vec{a}}$, which is invariant under the rigid body transformations. Screws can have finite or infinite pitches. For example, pure moments are infinite pitch screws given by $\vec{a} = \vec{0}$. If $h = 0$, the screw is called a zero pitch screw. Examples are pure forces and rotations.

Any scalar measure on a vector space can be defined by a *metric*. There is no positive definite metric in screw space that is geometrically or physically meaningful. Instead, the pitch is used as a scalar measure. If \vec{v} is any vector then a metric can be represented by a symmetric matrix G such that $\vec{v}^T G \vec{v}$ is a scalar measure. If G is definite then any non-zero vector has a non-zero scalar measure. If G is not definite, it is possible to have vectors whose scalar measure is zero. Such vectors are called *isotropic* vectors. For screws

the matrix

$$\hat{\Delta} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \quad (41)$$

where all submatrices are 3×3 , defines an indefinite metric. This is related to the pitch since $\frac{1}{2} \hat{S}^T \hat{\Delta} \hat{S} = \vec{a}^T \vec{b}$. Consequently, the zero and infinite pitch screws are the isotropic vectors of the screw space under this metric.

A set of $n \leq 6$ independent screws spans a subspace called an n -system of screws. An n -system may or may not contain isotropic screws. Now, if $\hat{V} = [\hat{S}_1, \dots, \hat{S}_n]$ is a matrix of basis screws, then any other screw in the n -system can be written as a linear combination $\hat{S} = \hat{V} \vec{u}$, where \vec{u} is an $n \times 1$ matrix of coefficients. Then, any isotropic screw \hat{S} must satisfy

$$\hat{S}^T \hat{\Delta} \hat{S} = \vec{u}^T (\hat{V}^T \hat{\Delta} \hat{V}) \vec{u} = 0 \quad (42)$$

The matrix $A = \hat{V}^T \hat{\Delta} \hat{V}$ is a symmetric matrix of order n . Every solution \vec{u} corresponds to an isotropic screw in the n -system. But, from (42), \vec{u} must be an isotropic vector of A by definition. So, by the existence theorem, such an n -system of screws contains zero or infinite pitch screws if and only if A is indefinite (non-trivial) or singular (trivial). If $A = 0$ then all the screws in the system are isotropic.

6.3 Stiffness Synthesis Problem

The spatial stiffness of a rigid body suspended by an elastic connection is represented by a 6×6 symmetric matrix \hat{K} , such that $\delta \hat{W} = \hat{K} \delta \hat{T}$, where $\delta \hat{T}$ is an infinitesimal twist and $\delta \hat{W}$ is an infinitesimal wrench. Ciblak and Lipkin [3] show that if \hat{K} has zero trace off-diagonal 3×3 submatrices, the synthesis of a stable or semi-stable stiffness by springs is reducible to the solutions of the equation

$$U^T (\hat{P}^T \hat{\Delta} \hat{P}) U = \Phi \quad (43)$$

where $\hat{K} = \hat{P} \hat{P}^T$, $\text{trace}(\hat{P}^T \hat{\Delta} \hat{P}) = 0$ and Φ is a symmetric matrix with zero diagonals. U is an orthogonal matrix. Clearly, the columns of U are the isotropic vectors of $A = \hat{P}^T \hat{\Delta} \hat{P}$. Since the previous section proved the existence of finitely or infinitely many orthonormal sets of isotropic vectors for any given zero trace matrix (Corollary 15), any stiffness can be synthesized by springs if and only if its off-diagonals have zero trace.

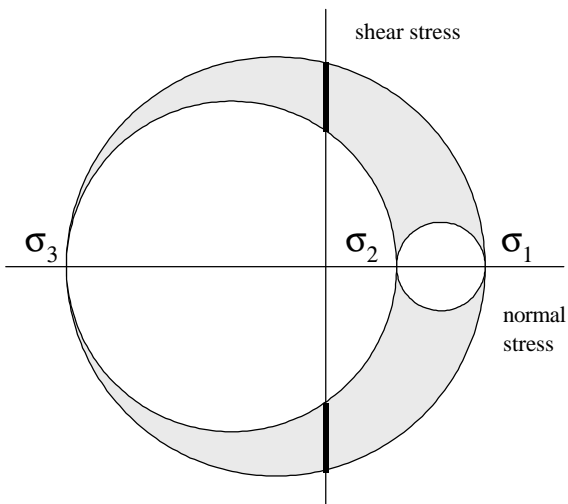


Figure 5. Mohr's circle for 3-dimensional deviatoric stress.

7 SUMMARY

The isotropic vector problem has complementary properties compared to the eigenvalue problem. Geometrically, the former is about orthogonality whereas the latter is about parallelism. From a functional point of view, the isotropic vectors are the zeros and the eigenvectors are the stationary points of the same quadratic form over a vector space.

Existence of the isotropic vectors basically requires indefiniteness. On the other hand, for the existence of an orthonormal basis formed by isotropic vectors it is necessary and sufficient that the matrix has zero trace. For a matrix of order n , the space of all orthonormal bases formed by isotropic vectors is $\frac{1}{2}(n-1)(n-2)$ dimensional in general.

The recursive algorithm presented for the construction of orthonormal bases formed by isotropic vectors is well suited for computer applications. Explicit solution of the three dimensional case is applicable to the synthesis of stiffness using three line springs and three torsional springs [4].

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