Introduction to Diffusion Tensor Imaging Mathematics: Part I. Tensors, Rotations, and Eigenvectors

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ABSTRACT: The mathematical aspects of diffusion tensor magnetic resonance imaging (DTMRI, or DTI), the measurement of the diffusion tensor by magnetic resonance imaging (MRI), are discussed in this three-part series. In part I, some general features of diffusion imaging are presented briefly, including the relationship between the diffusion ellipsoid and the diffusion tensor. Rotations of vectors and tensors are explained for both two and three dimensions. Rotationally invariant properties of the diffusion tensor are discussed. Calculation of the eigenvectors and eigenvalues of the diffusion tensor, which correspond to the directions of the diffusion ellipsoid axes and the squares of the hemiaxis lengths, is explained. Concepts Magn Reson Part A 28A: 101–122, 2006

KEY WORDS: diffusion; diffusion tensor; DTI; eigenvalues; eigenvectors; mathematics; rotational invariants; rotations; vectors

INTRODUCTION

Diffusion refers to the random (Brownian) motion of molecules in a fluid (liquid or gas). The relative amount of diffusion is expressed in terms of a parameter called the diffusion coefficient, D. In a homogeneous liquid such as water, the diffusion coefficient is the same in every direction, or isotropic. In some biological tissues the diffusion coefficient is different in different directions, or anisotropic. Diffusion tensor magnetic resonance imaging (DTMRI, or DTI), a method for measuring the relative diffusion coefficients of water molecules in different directions in each pixel of an MR image, involves diffusion-weighted imaging (DWI) measurements in at least six noncollinear directions (*1–13*). Measurements of diffusion anisotropy have been used to measure the structural integrity of brain white matter at different ages (*14*) and in several diseases (*15*, *16*). The direction of greatest diffusion has been used to follow white matter nerve fiber tracts, a process called tractography (*3*, *17–25*). Because DTI uses formulas that are not widely used elsewhere in NMR and MRI, the mathematics of DTI may not be familiar to MRI

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physicists, chemists, programmers, neuroscientists, students, and other researchers.

This series of three articles has several purposes:

1. To assemble in one place a large number of formulas that may be encountered in DTI.
2. To show how some formulas that may appear different are actually equivalent.
3. To point out and correct some published mistakes.
4. To explain the relationship between the diffusion ellipsoid and the diffusion tensor.
5. To show how to calculate diffusion-weighting factors (*b* factors).
6. To explain how to calculate tensor elements, eigenvalues, and eigenvectors from experimental data (MRI signal intensities).
7. To discuss the effects of noise on DTI measurements and calculations.
8. To explain how to simulate DTI measurements.
9. To discuss how to optimize DTI acquisition parameters by propagation-of-error calculations and by simulations.

These articles will not discuss fiber tract mapping (tractography), correction of image artifacts (induced by eddy currents or by magnetic susceptibility differences), or the reasons that DWI signal decay should be monoexponential (*26*) or biexponential (*27–33*).

This series of articles assumes that the reader 1) knows something about DTI theory or applications and wants to learn more; 2) is familiar with vectors; 3) understands basic matrix mathematics, including multiplication, transposition, and inversion; and 4) is familiar with basic MRI concepts such as spin echoes and echo planar imaging (EPI). These articles do not assume familiarity with tensors, eigenvalues, eigenvectors, or anisotropy. Although this series focuses on diffusion tensor imaging, the concepts are equally applicable to nonimaging NMR measurements of diffusion.

Diffusion tensor imaging mathematics assumes monoexponential signal decay as the diffusion-weighting factor, *b*, increases. The diffusion process can be described by Fick's laws of diffusion (*18*, *34*). An excellent derivation of the expected monoexponential signal decay from Fick's laws of diffusion has appeared in this journal (*26*) and will not be repeated here. Monoexponential signal decay requires that diffusion is uniform in each direction, without sudden restrictions or hindrances. Furthermore, there is a single fiber type and orientation in each pixel. Although biexponential signal decay has been detected at high *b* factors in biological systems (*27–33*), DTI is still useful at low to moderate *b* factors for anisotropy measurements and tractography.

Some DTI concepts and formulas are easier to visualize and understand in two dimensions than in three dimensions (*35*). Therefore, some things will be explained in two dimensions, and then the corresponding three-dimensional (3D) formulas will be presented. This involves the use of 2×2 tensors that describe ellipses and 3×3 tensors that describe ellipsoids.

In this first part of this series, vectors and tensors are introduced in two dimensions (2D) and three dimensions, and their rotations are discussed. Rotationally invariant properties of the tensor are described. The calculation of eigenvectors and eigenvalues from the tensor is explained. A list of errors in DTI-related publications is included as an appendix. Part II discusses diffusion anisotropy indices (DAIs), explains how the diffusion-weighting *b* factor is calculated, and explores different gradient sampling schemes for DWI and DTI. Part III explains how the tensor is calculated from DWI data in six or more directions, discusses computer simulations and the effects of noise on DTI measurements, and explores the optimization of DTI data acquisition and processing.

Introductory material on DWI and DTI is available in many journal articles (*1–3*, *36*, *37*) and book chapters (*18*, *34*). Entire journal issues devoted to diffusion imaging include the November/December issues (no. 7/8) of volumes 8 (*1995*) and 15 (*2002*) of *NMR in Biomedicine*, and the March issue (no. 3) of volume 45 (*2003*) of *European Journal of Radiology*.

DIFFUSION SPHERES, ELLIPSOIDS, AND PEANUTS

The purposes of this section are to explain 1) a little bit about the diffusion process and 2) how we visualize the diffusion process by an ellipsoid that shows the root mean squared displacement in each direction, and by a "peanut" that shows the apparent diffusion coefficient that would be measured in each direction.

Over time, a molecule that begins at a certain point in a homogeneous fluid will move randomly so that at a later time, t, it will, on the average, be some distance away from where it started. If we measured the probability of finding the molecule at various distances in each direction, we could choose the point in each direction that represents the root mean squared displacement in that direction (*5*, *18*). These points would form a sphere with radius $\sqrt{2Dt}$, where D is the diffusion coefficient. The units of D are distance^2/time (e.g., $\mu m^2/s$), and the units of Dt are distance^2(e.g., μm^2). A smaller diffusion coefficient or time results in a smaller sphere, and a larger diffusion coefficient or time results in a larger sphere (*5*).

In biological systems the measured diffusion coefficient is influenced by proteins, membranes, and other biological molecules. In addition, there may be multiple nonexchanging or slowly exchanging compartments. The measured value of the diffusion coefficient generally depends on the diffusion time and on the amount of diffusion weighting factor, b. Therefore, no single value of D fully characterizes the diffusion process. In such cases diffusion is expressed as the apparent diffusion coefficient (*ADC*), which is also represented by the letter D. Furthermore, diffusion is often anisotropic, so the measured *ADC* depends on the measurement direction. Anisotropic diffusion is modeled as a diffusion ellipsoid, with possibly different hemiaxis lengths (which are proportional to the square roots of the tensor eigenvalues, $\lambda_1 > \lambda_2 > \lambda_3$) along three orthogonal axes (which correspond to the tensor eigenvectors $\boldsymbol{\varepsilon}_1$, $\boldsymbol{\varepsilon}_2$, $\boldsymbol{\varepsilon}_3$). Good pictures of diffusion ellipsoids are available from several sources (*3–5*, *18*, *19*, *38–40*). In the (x', y', z') reference frame whose axes are parallel to the principal axes (eigenvectors) of the ellipsoid, which has been called the "principal frame" or the "principal axis system," the ellipsoid equation is (*3–5*)

$$\frac{x'^2}{2\lambda_{x'}t} + \frac{y'^2}{2\lambda_{y'}t} + \frac{z'^2}{2\lambda_{z'}t} = 1 \qquad [1]$$

Some previous work has used the (x, y, z) reference frame to represent the laboratory reference frame, where the ellipsoid has some arbitrary orientation, and the (x', y', z') reference frame to represent the principal axis system of the ellipsoid. In the present work the (x', y', z') reference frame sometimes refers to an arbitrary ellipsoid orientation.

As with the isotropic diffusion sphere, the anisotropic diffusion ellipsoid represents the root mean squared displacement in each direction. Plotting the *ADC* in each direction generally results in a peanut-shaped curve rather than an ellipse. In each direction the measured D is determined by the projections of the three eigenvectors onto a unit vector, $\mathbf{v}$, in the chosen direction (*38*, *41*). Each projection is given by the dot product between the eigenvector and $\mathbf{v}$ (an example of a dot product will be shown in Eq. [3]).

$$D = \mathbf{v}^{\mathrm{T}}\mathbf{D}\mathbf{v} = \lambda_1(\mathbf{v}\cdot\varepsilon_1)^2 + \lambda_2(\mathbf{v}\cdot\varepsilon_2)^2 + \lambda_3(\mathbf{v}\cdot\varepsilon_3)^2 \qquad [2]$$

If $\mathbf{v}$ is one of the eigenvectors, only one of the $\mathbf{v} \cdot \boldsymbol{\varepsilon}$ terms is nonzero, and the measured D is the corresponding eigenvalue λ. Some 2D examples are shown in Fig. 1. In each example the dotted ellipse shows the root mean squared displacement ($\sqrt{2Dt}$) in each direction, while the solid peanut-shaped curve shows the D that would be measured in each direction (*35, 38, 42*). Because of the different units in D and the ellipse, the ellipse has been scaled to fit onto the same plots as D.

The diffusion ellipsoid is represented mathematically by a tensor. The tensor is most commonly represented by a symmetric 3×3 matrix. For some mathematical formulas it is more convenient to represent the tensor elements as a vector. Although a discussion of general tensor properties is beyond the scope of this introductory series, it is worth mentioning that the transformation of the diffusion tensor between two reference frames can be calculated with the same rotation matrices that describe vector transformations. Therefore, knowledge of vector rotation matrices will be useful in understanding tensor rotations.

After learning how ellipses and ellipsoids are described by tensors, we investigate some of the properties of the tensor. More information on the relationship between the diffusion tensor and the diffusion ellipse is available in (*5*, *18*).

VECTORS AND VECTOR ROTATIONS

The purpose of this section is to derive the formulas that describe the rotation of an object, represented by a vector, in a fixed reference frame (coordinate system), or that express a fixed vector in reference frames that are rotated with respect to each other.

Vectors

A vector has magnitude (length) and direction. Vectors are usually assumed to be column vectors, and may be written as the transpose of a row vector. For example, if (x, y, z) is a row vector, its transpose, $(x, y, z)^{\mathrm{T}}$, is a column vector. If $\mathbf{V}$ is the column vector $(x, y, z)^{\mathrm{T}}$, then $\mathbf{V}^{\mathrm{T}}$ is the row vector (x, y, z). Thus, the superscript T always indicates "transpose," but the transposed vector may be a column vector or a row vector, depending on the context. Sometimes the uppercase 'T' is typeset as a lowercase 't' or as a dagger, †.

Movement in a given direction can be represented by a vector from the origin to the final point, for example from $(0, 0)^{\mathrm{T}}$ to $(5, 0)^{\mathrm{T}}$ (Fig. 2). Movement in the opposite direction can be represented by a vector pointing in the opposite direction, for example from $(0, 0)^T$ to $(-5, 0)^T$ (see Fig. 2) or from $(5, 0)^T$ to $(0, 0)^T$. A vector can be moved around in the *xy* plane as long as the magnitude and direction remain the same.

A vector can be represented by giving its projections on the *x* and *y* axes. For example, the vector $(5, 0)^T$ has magnitude 5, its projection on the *x* axis is 5, and its projection on the *y* axis is 0 (see Fig. 2). The

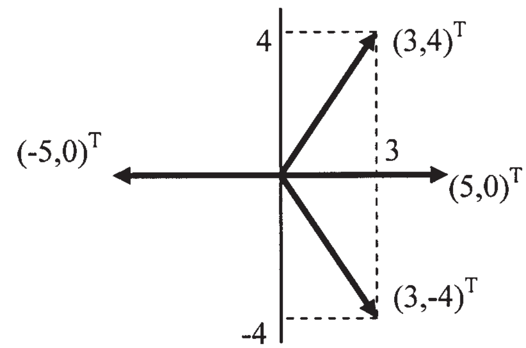

Figure 2 Examples of several vectors, each with magnitude 5.

vector $(3, 4)^T$ has magnitude 5, its projection on the *x* axis is 3, and its projection on the *y* axis is 4 (see Fig. 2). The vector $(3, -4)^T$ has magnitude 5, its projection on the *x* axis is 3, and its projection on the *y* axis is -4 (see Fig. 2). The sum of the *x* and *y* components changes as the vector is rotated in the *xy* plane, while the sum $x^2 + y^2$ remains the same. In other words, the sum $x^2 + y^2$ is rotationally invariant, whereas the sum $x + y$, or even $|x| + |y|$, is rotationally variant.

The vector components depend only on the relationship between the vector and the coordinate system. For example, the vectors in Figs. 3(a) and (c) are both represented by $(5, 0)^T$ because the projections of each vector on the *x* and *y* axes are 5 and 0, respectively, even though the coordinate axes (and vectors) in Fig. 3(c) are tilted with respect to Fig. 3(a).

Vector multiplication can produce two different results. If **u** and **v** are column vectors, then the product $\mathbf{u}^T\mathbf{v}$ is the dot product (inner product) of the vectors

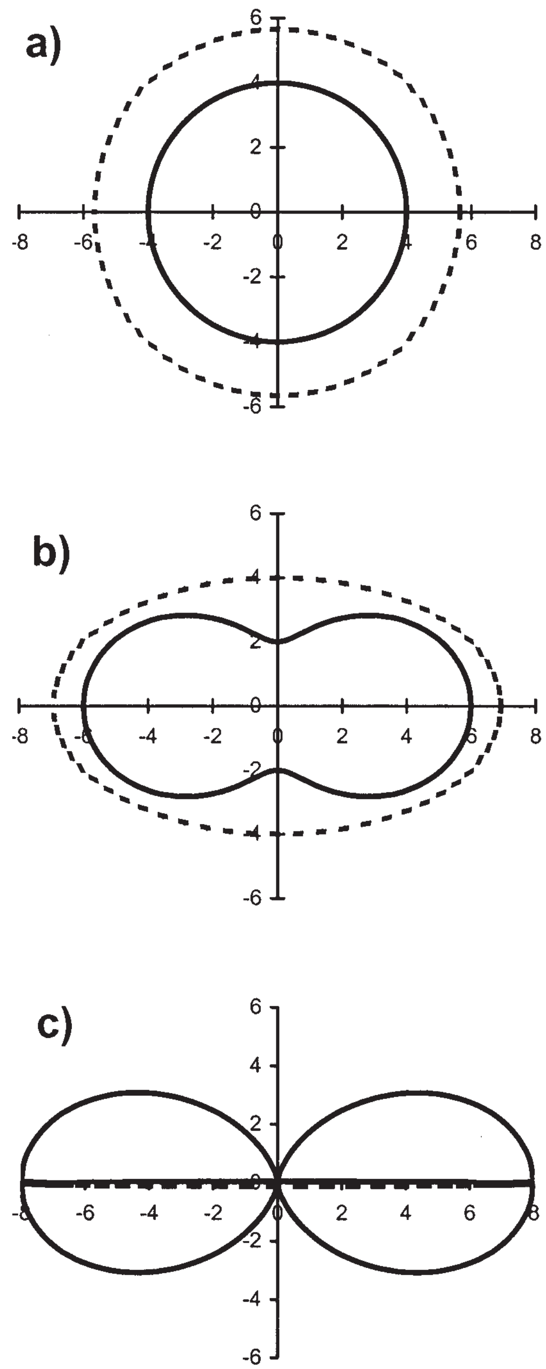

Figure 1 Examples of 2D diffusion ellipses and *ADC* "peanuts." In each case the dotted shape shows the root mean squared displacement ($\sqrt{2Dt}$) in each direction, and the solid shape shows the *ADC* that would be measured in that direction with $t = 1/2$. The trace of the tensor has the same value in each of the three cases shown. Because $\sqrt{2Dt}$ and *D* have different units, the ellipse has been scaled to fit onto the *ADC* plots. All ellipses are plotted with the same scale, and all "peanuts" are plotted with the same scale. (a) Isotropic diffusion, with *ADC* = 4 in each direction. The ellipse and the *ADC* "peanut" have spherical shapes. (b) Anisotropic diffusion, with *ADC* = 6 in the *x* direction and 2 in the *y* direction. (c) Unidirectional diffusion, with *ADC* = 8 in the *x* direction and 0 in the *y* direction. Although there is no diffusion in the *y* direction, a measurement anywhere but along the *y* axis results in a nonzero measured *ADC* given by the projection of diffusion in the *x* direction onto the chosen direction (Eq. [2]).

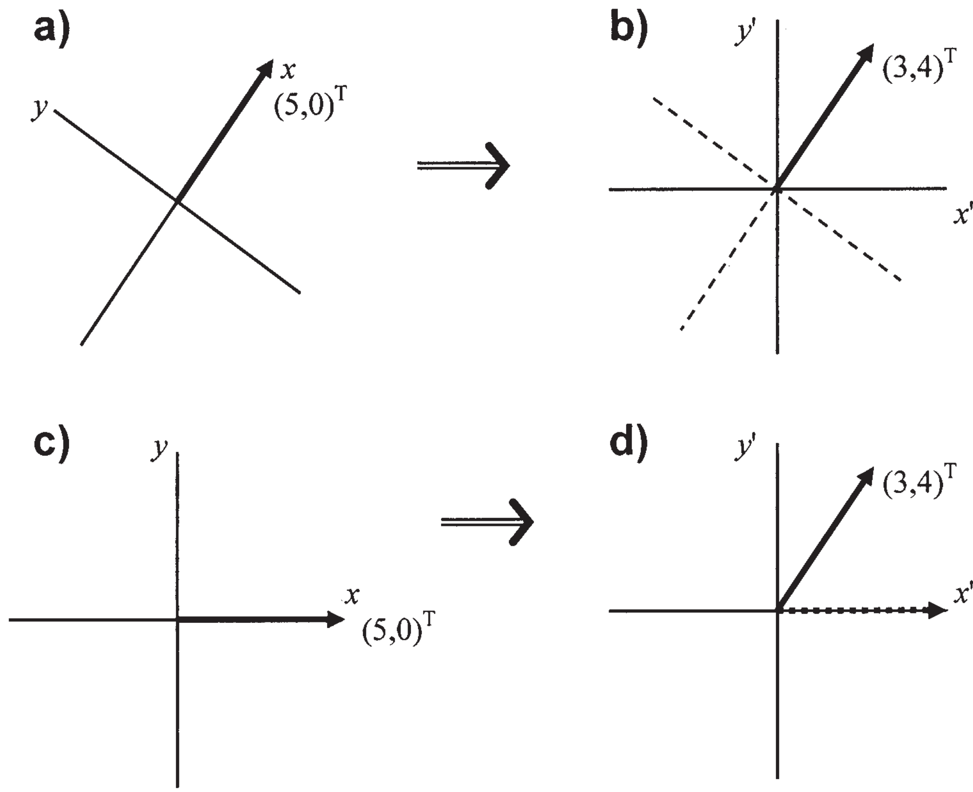

Figure 3 Visualization of 2D vector rotation. (a) and (b) Visualization of the reference frame rotating while the vector stays in place. The vector $(5, 0)^{\mathrm{T}}$ along the x axis in (a) becomes the vector $(3, 4)^{\mathrm{T}}$ after the reference frame rotates through an angle $-\theta$. (c) and (d) Visualization of the vector rotating in a fixed reference frame. The vector $(5, 0)^{\mathrm{T}}$ along the x axis in (c) rotates through an angle θ to the position $(3, 4)^{\mathrm{T}}$ in a fixed xy reference frame.

$$\mathbf{u}^{\mathrm{T}}\mathbf{v} = \mathbf{v}^{\mathrm{T}}\mathbf{u} = \mathbf{u}\cdot\mathbf{v} = \mathbf{v}\cdot\mathbf{u} = \begin{pmatrix} u_x & u_y & u_z \end{pmatrix}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} v_x & v_y & v_z \end{pmatrix}\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = u_xv_x + u_yv_y + u_zv_z \quad [3]$$

In contrast, $\mathbf{uv}^{\mathrm{T}}$ yields a 3×3 matrix:

$$\mathbf{uv}^{\mathrm{T}} = \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}\begin{pmatrix} v_x & v_y & v_z \end{pmatrix} = \begin{pmatrix} u_xv_x & u_xv_y & u_xv_z \\ u_yv_x & u_yv_y & u_yv_z \\ u_zv_x & u_zv_y & u_zv_z \end{pmatrix} \quad [4]$$

If $\mathbf{u} = \mathbf{v}$, this matrix is called a dyadic tensor (*41*).

Vector Rotation in Two Dimensions

Physicists conventionally consider an object to be fixed in space, while the observer can choose an arbitrary reference frame (coordinate system). A rotation is described as rotating a coordinate system relative to an object (see Fig. 3[a]). However, a vector also may change over time with respect to a fixed reference frame. For example, MR physicists and spectroscopists are accustomed to visualizing vectors moving from the z axis to the xy plane, and then precessing in the xy plane, of a reference frame that is rotating near the Larmor frequency. In this visualization the reference frame is fixed, and the isochromat vectors move. For example, rotation of a reference frame through an angle $-\theta$ (see Figs. 3[a] and [b]) can be visualized as rotating a vector through an angle $+\theta$ (see Figs. 3[c] and [d]). Mathematically, the two methods produce the same result: the vector $(5, 0)^{\mathrm{T}}$ before the rotation becomes $(3, 4)^{\mathrm{T}}$ after the rotation. We begin by looking at 2D vectors, and then progress to 3D vectors.

Consider the vectors $(3, -4)^{\mathrm{T}}$ and $(5, 0)^{\mathrm{T}}$ in Figs. 4 and 5. An off-axis vector can be represented as the sum of an x-axis vector plus a y-axis vector, for example (see Figs. 4 and 5):

$$(3, -4)^{\mathrm{T}} = (3, 0)^{\mathrm{T}} + (0, -4)^{\mathrm{T}} \quad [5]$$

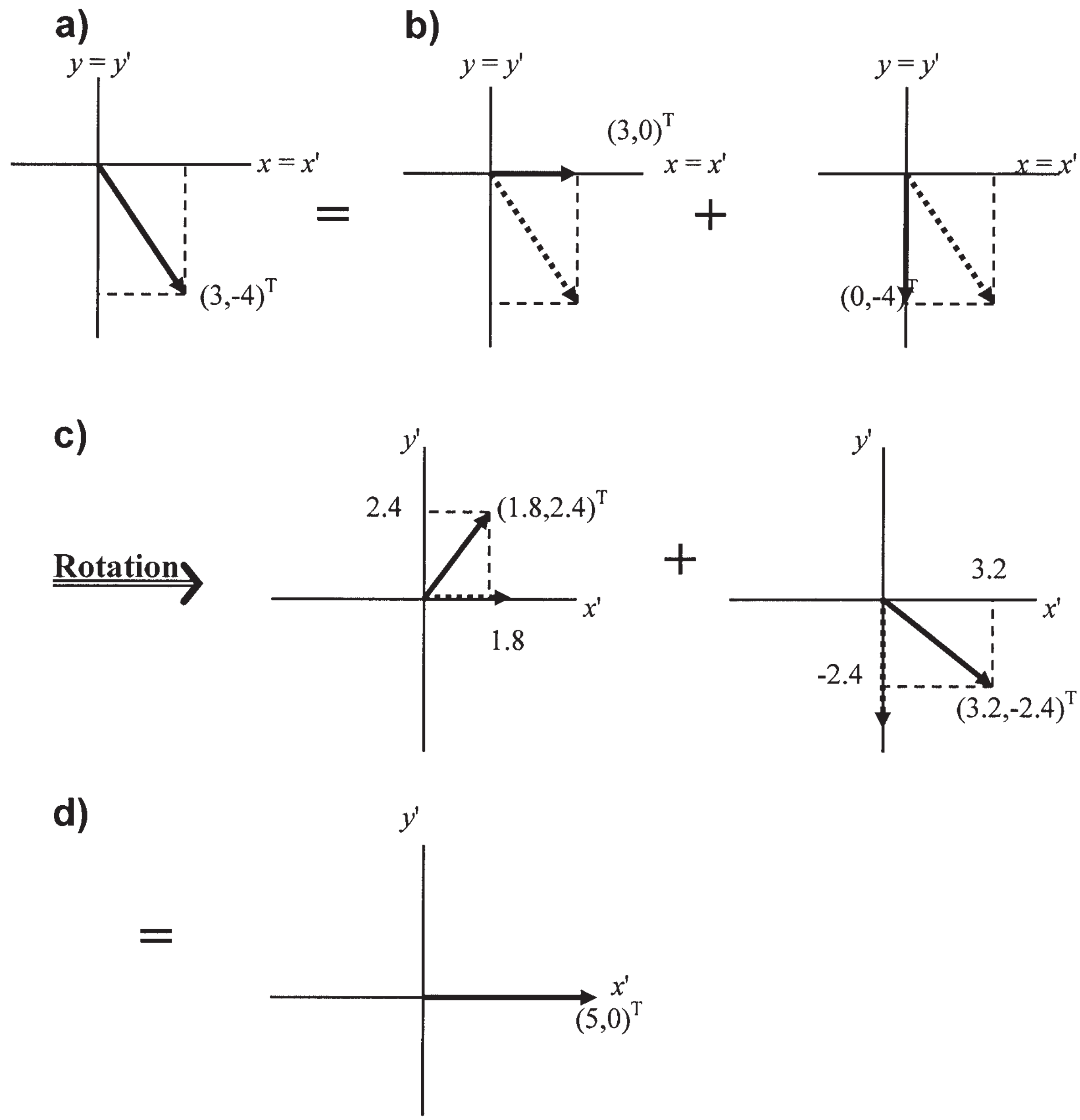

Figure 4 Calculating a 2D vector rotation by calculating the effect on each individual component. The rotation is visualized as the vector rotating in a fixed *xy* reference frame. The vector $(3, -4)^T$ in (a) can be decomposed into *x* and *y* components, $(3, 0)^T$ and $(0, -4)^T$ in (b). In (c), each component vector rotates through an angle θ, resulting in new *x* and *y* components. (d) The resultant *x* and *y* components are summed to yield the final result $(5, 0)^T$.

In general,

$$\mathbf{V} = \mathbf{V}_x + \mathbf{V}_y = (V_x, 0)^T + (0, V_y)^T \qquad [6]$$

The formula for the result of rotating the reference frame with respect to a vector **V** can be derived by considering the effect on each individual component of **V** (see Figs. 4 and 5). If the vector $(3, -4)^T$ is the starting point and $(0, 5)^T$ is the end point, the angular difference between them is θ, where $\sin\theta = 0.8$ and $\cos\theta = 0.6$. Rotation of the reference frame through an angle $-\theta$ (see Fig. 5) can be represented by a rotation matrix, which is

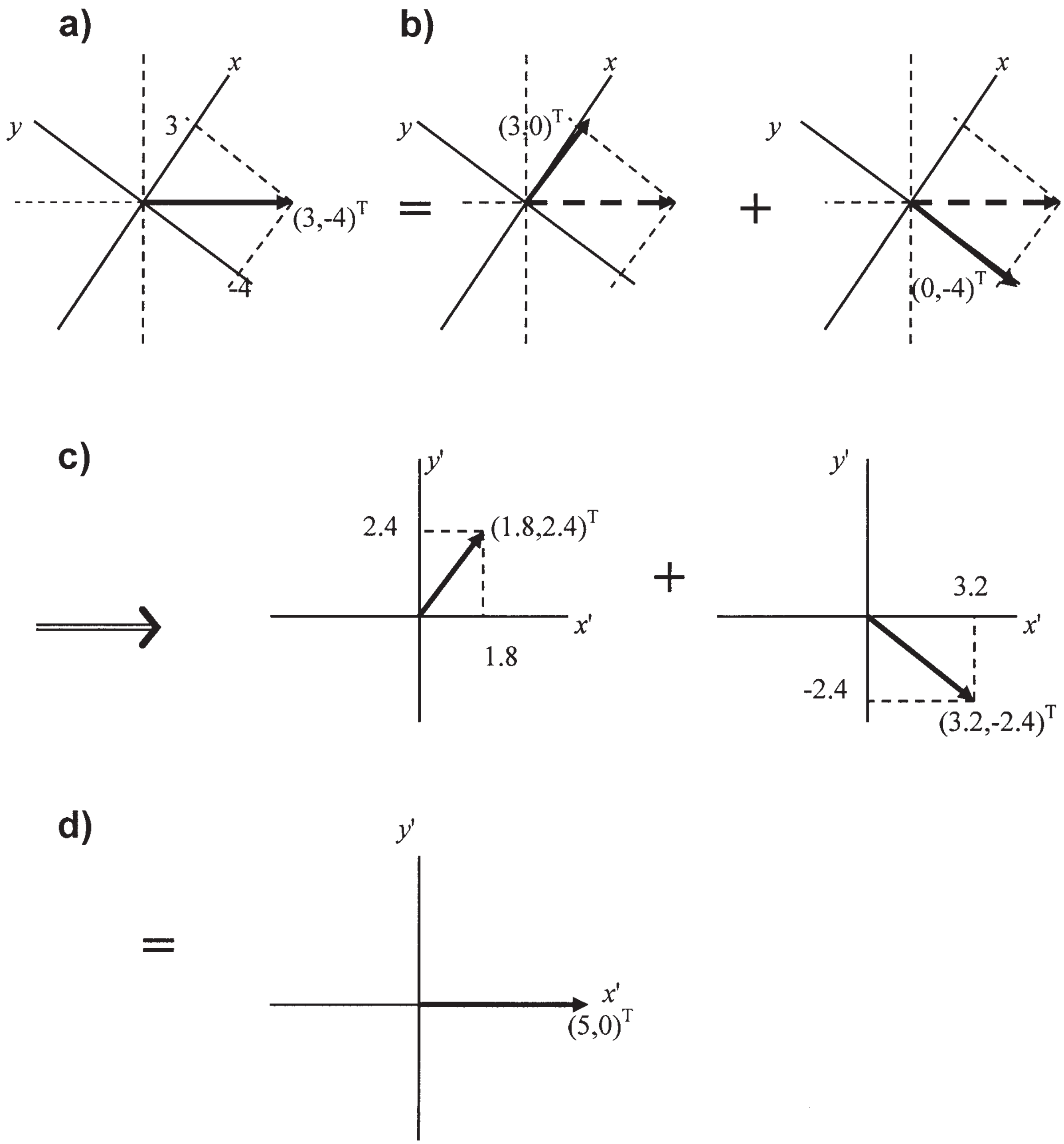

Figure 5 Calculating a 2D vector rotation by calculating the effect on each individual component. The rotation is visualized as the vector staying in place while the *xy* reference frame rotates. The vector $(3, -4)^T$ in (a) can be decomposed into *x* and *y* components, $(3, 0)^T$ and $(0, -4)^T$ in (b). In (c), the reference frame of each component vector rotates through an angle $-\theta$, resulting in new *x* and *y* components. (d) The resultant *x* and *y* components are summed to yield the final result $(5, 0)^T$.

designated $\mathbf{R}(-\theta)$. When the object (in this case, a vector) is visualized as being rotated through an angle θ (see Fig. 4), the rotation matrix is designated $\mathbf{R}_o(\theta)$, and clearly

$$\mathbf{R}(-\theta) = \mathbf{R}_o(\theta) \qquad [7]$$

Consider the visualization of the vector rotating through an angle θ in a fixed reference frame (see Fig. 4[c]). Thus, V_x along the *x* axis becomes $V_x \cos\theta$ along the *x* axis plus $V_x \sin\theta$ along the *y* axis. Similarly, V_y along the *y* axis becomes $V_y \cos\theta$ along the *y* axis plus $-V_y \sin\theta$ along the *x* axis.

$$V_x\hat{\mathbf{i}} = 3\hat{\mathbf{i}} \rightarrow V_x\cos\theta\hat{\mathbf{i}} + V_x\sin\theta\hat{\mathbf{j}} = 1.8\hat{\mathbf{i}} + 2.4\hat{\mathbf{j}} \quad [8]$$

$$V_y\hat{\mathbf{j}} = -4\hat{\mathbf{j}} \rightarrow V_y\cos\theta\hat{\mathbf{j}} - V_y\sin\theta\hat{\mathbf{i}} = -2.4\hat{\mathbf{j}} + 3.2\hat{\mathbf{i}} \quad [9]$$

where $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$ are unit vectors along the x and y axes, respectively. The new vector coordinates (V'_x, V'_y) are found by summing the components on each axis, $\hat{\mathbf{i}}$ for V'_x and $\hat{\mathbf{j}}$ for V'_y (see Fig. 4[d]):

$$V'_x = V_x\cos\theta - V_y\sin\theta = 1.8 + 3.2 = 5 \quad [10]$$

$$V'_y = V_x\sin\theta + V_y\cos\theta = 2.4 - 2.4 = 0 \quad [11]$$

We can represent this rotation by a rotation matrix $\mathbf{R}_o(\theta)$, so that $\boldsymbol{V}' = \mathbf{R}_o(\theta)\boldsymbol{V}$:

$$\mathbf{V}' = \begin{pmatrix} V'_x \\ V'_y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} V_x \\ V_y \end{pmatrix} = \mathbf{R}_o(\theta)\mathbf{V} \quad [12]$$

We can derive the same equation by visualizing the reference frame as rotating through an angle $-\theta$ relative to the vector (Fig. 5). Thus, $\mathbf{R}_o(\theta) = \mathbf{R}(-\theta)$, consistent with Eq. [7].

The transpose of this rotation matrix is also its inverse and corresponds to rotation in the opposite direction:

$$\mathbf{R}(\theta) = \mathbf{R}_o(-\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \quad [13]$$

$$\mathbf{R}(-\theta) = \mathbf{R}_o(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad [14]$$

$$\mathbf{R}^{\mathrm{T}}(\theta) = \mathbf{R}^{-1}(\theta) = \mathbf{R}(-\theta) = \mathbf{R}_o(\theta) \quad [15]$$

Because most people find it easier to visualize a fixed reference frame and a moving vector, the examples below use that convention. Keep in mind that, technically, it is the reference frame that moves, not the vector. Phrases such as "after rotation through an angle θ" can be confusing, because it is not clear whether the reference frame rotated through the angle θ, or the vector rotated through the angle θ. To avoid confusion, one can give the actual rotation matrices, state the initial and final vector positions, or specify whether the reference frame or vector rotated though the angle θ.

Vector Rotation in Three Dimensions

In three dimensions, a rotation axis must be specified. In two dimensions, the rotation is implicitly about the z axis. Rotation of a reference frame by an angle $-\theta$ about the x, y, or z axis is given by the following matrices:

$$\mathbf{R}(x, -\theta) = \mathbf{R}_o(x, \theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \quad [16]$$

$$\mathbf{R}(y, -\theta) = \mathbf{R}_o(y, \theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \quad [17]$$

$$\mathbf{R}(z, -\theta) = \mathbf{R}_o(z, \theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad [18]$$

A few properties of rotation matrices are worth mentioning. First, the transpose of a rotation matrix equals the inverse of the matrix, $\mathbf{R}^{\mathrm{T}} = \mathbf{R}^{-1}$ (Eq. [15]). This is true because the column vectors of a rotation matrix form an orthonormal set—each vector has a magnitude = 1 (the dot product of each vector with itself = 1), and the dot product with the other two vectors equals 0—and the row vectors form a different orthonormal set. Thus, the consecutive application of a rotation and its transpose (its inverse) produces no net effect:

$$\mathbf{R}\mathbf{R}^{-1} = \mathbf{R}^{-1}\mathbf{R} = \mathbf{R}\mathbf{R}^{\mathrm{T}} = \mathbf{R}^{\mathrm{T}}\mathbf{R} = \mathbf{I} \quad [19]$$

where $\mathbf{I}$ is the identity matrix (1s along the diagonal, 0s elsewhere).

Second, the inverse of a multiple-rotation operation, for example $\mathbf{R}_1\ \mathbf{R}_2$, is the inverse operations performed in the reverse order:

$$(\mathbf{R}_1\mathbf{R}_2)^{-1} = (\mathbf{R}_1\mathbf{R}_2)^{\mathrm{T}} = \mathbf{R}_2^{-1}\mathbf{R}_1^{-1} = \mathbf{R}_2^{\mathrm{T}}\mathbf{R}_1^{\mathrm{T}} \quad [20]$$

because

$$\mathbf{R}_2^{-1}\mathbf{R}_1^{-1}\mathbf{R}_1\mathbf{R}_2 = \mathbf{R}_1\mathbf{R}_2\mathbf{R}_2^{-1}\mathbf{R}_1^{-1} = \mathbf{I} \quad [21]$$

Third, when two or more rotations are performed consecutively, a single overall rotation matrix can be determined by multiplying the matrices together. The matrix representing the first rotation is on the right, and the subsequent rotation matrices are added on the left. For example, if a rotation is visualized as the vector rotating first about the y axis through an angle θ, then about the z axis through an angle ϕ, the overall rotation matrix is $\mathbf{R}_o(z, \phi)\ \mathbf{R}_o(y, \theta) = \mathbf{R}(z, -\phi)\ \mathbf{R}(y, -\theta)$, and application of Eqs. [17] and [18] yields

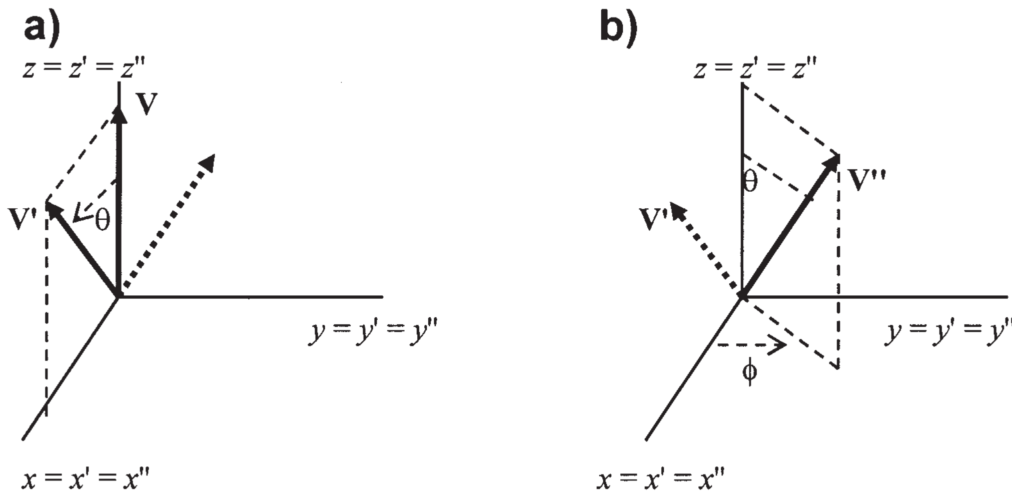

Figure 6 Three-dimensional rotation visualized as a vector rotating in a fixed *xy* reference frame. (a) From the *z* axis, the vector **V** rotates about *y* axis by angle θ, becoming the vector **V**′. (b) The vector **V**′ rotates about *z* axis by angle ϕ to the final position, **V**″.

$$\mathbf{R}(z,-\varphi)\mathbf{R}(y,-\theta) = \begin{pmatrix} \cos\varphi\cos\theta & -\sin\varphi & \cos\varphi\sin\theta \\ \sin\varphi\cos\theta & \cos\varphi & \sin\varphi\sin\theta \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \quad [22]$$

Equation [20] shows that the transpose of this matrix is

$$[\mathbf{R}(z,-\phi)\mathbf{R}(y,-\theta)]^{\mathrm{T}} = \mathbf{R}(y,\theta)\mathbf{R}(z,\phi) \quad [23]$$

which represents the reverse rotations in reverse order. Therefore, the matrix for the *same* rotations performed in the reverse order is the transpose of the original rotation matrix with the angles θ, ϕ replaced by negative angles −θ, −ϕ:

$$\mathbf{R}(y,-\theta)\mathbf{R}(z,-\phi) = [\mathbf{R}(z,\phi)\mathbf{R}(y,\theta)]^{\mathrm{T}} \quad [24]$$

$$\mathbf{R}(y,-\theta)\mathbf{R}(z,-\varphi) = \begin{pmatrix} \cos\theta\cos\varphi & -\cos\theta\sin\varphi & \sin\theta \\ \sin\varphi & \cos\varphi & 0 \\ -\sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \end{pmatrix} \quad [25]$$

In general, $\mathbf{R}_1\,\mathbf{R}_2$ is not equal to $\mathbf{R}_2\,\mathbf{R}_1$ unless the same rotation axis is used in both cases, or one rotation is through an angle of $2n\pi$, where n is an integer.

Fourth, after a rotation matrix is applied to a vector aligned along one of the orthogonal axes (*x*, *y*, or *z*), the resulting vector is parallel to the corresponding column vector of the rotation matrix. In this example, after the rotation operation $\mathbf{R}(z,-\phi)\,\mathbf{R}(y,-\theta)$ (Eq. [22]), the vector $(1, 0, 0)^{\mathrm{T}}$ becomes $(\cos\phi\cos\theta, \sin\phi\cos\theta, -\sin\theta)^{\mathrm{T}}$; the vector $(0, 1, 0)^{\mathrm{T}}$ becomes $(-\sin\phi, \cos\phi, 0)^{\mathrm{T}}$; and the vector $(0, 0, 1)^{\mathrm{T}}$ becomes $(\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)^{\mathrm{T}}$.

Rotation of a Vector to a Desired Position Specified by Angles

Consider the problem of finding the rotation matrix such that a vector **V** originally aligned with the *z* axis (Fig. 6[a]) will become the vector **V**″, so that **V**″ will form an angle θ with the *z*″ axis, and its projection in the *x*″*y*″ plane will form an angle ϕ with the *x*″ axis (see Fig. 6). This rotation matrix is given in Eq. [22]. To calculate this result, one option is to visualize the vector **V** rotating through an angle θ about the *y* axis so that **V**′ lies in the *x*′*z*′ plane (see Fig. 6[a]), $\mathbf{R}_o(y, \theta)$, then rotating **V**′ through an angle ϕ about the *z*′ axis (see Fig. 4), $\mathbf{R}_o(z, \phi)$. This yields $\mathbf{R}_o(z,\phi)\,\mathbf{R}_o(y,\theta)$, and application of Eq. [7] shows that this equals $\mathbf{R}(z,-\phi)\,\mathbf{R}(y,-\theta)$. There are other ways to visualize this rotation, and they all give the same mathematical result.

Rotation of a Vector to a Desired Position Specified by Cartesian Coordinates

The discussion so far has focused on formulas for rotation through a known angle about a specified axis of an orthogonal coordinate system. A vector can be rotated to any desired position by the application of two properly selected rotations. To rotate a vector from any given axis, say the *z* axis, to a desired position, it is only necessary that the corresponding column (in this case, the third column) of the rotation matrix be parallel to the desired ending position. The other two columns must complete the orthonormal set, resulting in an infinite set of rotation matrices that will accomplish the desired rotation. It is also possible to specify that a vector along another axis, say the x axis, be simultaneously rotated to another specified position, as long as it remains orthogonal to the vector that began on the z axis. The third axis of the rotated reference frame will be given by the proper cross product of the first two axes ($x = y \times z$, $y = z \times x$, $z = x \times y$). For example, if a vector along the z axis is to end up at $(2/3, 2/3, 1/3)^T$, and a vector along the x axis is to end up at $(1/2)(-2^{1/2}, 2^{1/2}, 0)^T$, then a vector along the y axis will end up at $(2^{1/2}/6)(-1, -1, 4)^T$, and the rotation matrix is given by

$$\mathbf{R} = \begin{pmatrix} -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{6} & 2/3 \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{6} & 2/3 \\ 0 & \frac{2\sqrt{2}}{3} & 1/3 \end{pmatrix} \qquad [26]$$

The rotation matrix in Eq. [26] is one possible rotation matrix that moves a vector from the z axis to the desired position. Other possible rotation matrices would correspond to an initial rotation about the z axis by some angle Ψ. This rotation would not affect the vector along the z axis but would mix the x and y axes so that vectors initially aligned with the x or y axis would end up in different positions.

Important Points in "Vectors and Vector Rotations"

The 2D rotation matrices are in Eqs. [13] and [14]. The 3D rotation matrices are in Eqs. [16–18]. The transpose of a rotation matrix is its inverse (Eqs. [15], [19], and [20]). Rotations about more than one axis can be expressed as a series of individual rotations (as in Eq. [22]), or by a rotation matrix whose columns are the desired final position of a vector starting on the x, y, or z axis (as in Eq. [26]). The inverse of a multiple-rotation operation is the set of inverse operations performed in the reverse order (Eq. [20]).

TENSORS AND TENSOR ROTATIONS

The purposes of this section are 1) to explain how the rotation matrices that were derived for vectors can be used to describe the rotation of an object, represented by a tensor, in a fixed reference frame (coordinate system), or to express a fixed tensor in reference frames that are rotated with respect to each other; and 2) to show formulas for some rotationally invariant properties of the tensor that will be used to evaluate and compare tensors, including the mean diffusivity and the degree of anisotropy.

Tensors

As discussed above, the diffusion ellipsoid is represented by a tensor, which can be expressed as a symmetric 3×3 matrix. Although the diffusion ellipsoid can be represented by the three tensor eigenvectors (ellipsoid axis directions) and their associated eigenvalues (which are proportional to the squares of the ellipsoid hemiaxis lengths), these are not measured directly. Instead, we measure the tensor and then derive the eigenvalues and eigenvectors from the tensor.

The three orthogonal axes of the ellipsoid could be aligned with the x, y, and z axes of the reference frame, or the ellipsoid could be tilted with respect to two or three axes. Rotation of the ellipsoid by 180° about any principal axis produces an equivalent ellipsoid. In two dimensions, a diffusion ellipse can be aligned with the x and y axes, or it can be tilted. The mathematical representation of the ellipsoid (or ellipse) must include information about the lengths of the axes and their spatial orientation.

When a diffusion ellipsoid (or ellipse) is aligned with the reference frame axes (the principal axis system), the tensor describing the ellipsoid (ellipse) is diagonal. The diagonal elements, which are the eigenvalues of the tensor, denoted by λ, are proportional to the squares of the lengths of the ellipsoid (ellipse) axes. This was explained in the text around Eq. [2]. When the ellipsoid (ellipse) is rotated with respect to the reference frame, off-diagonal elements appear.

Tensor Rotation in Two Dimensions

Tensor rotation involves multiplication on the left by a rotation matrix and on the right by the transpose (inverse) of the rotation matrix:

$$\begin{pmatrix} D'_{xx} & D'_{xy} \\ D'_{yx} & D'_{yy} \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} D_{xx} & D_{xy} \\ D_{xy} & D_{yy} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad [27]$$

Expansion of Eq. [27] yields

$$D'_{xx} = a^2 D_{xx} + c^2 D_{yy} + 2ac D_{xy} \qquad [28]$$

$$D'_{xy} = D'_{yx} = (ad + bc)\,D_{xy} + abD_{xx} + cdD_{yy} \quad [29]$$

$$D'_{yy} = d^2D_{yy} + b^2D_{xx} + 2bdD_{xy} \quad [30]$$

Consider a 2D diffusion ellipse aligned with the x and y axes, with $D_x = 6$ and $D_y = 2$. This can be represented by the tensor

$$\begin{pmatrix} D_{xx} & D_{xy} \\ D_{xy} & D_{yy} \end{pmatrix} = \begin{pmatrix} 6 & 0 \\ 0 & 2 \end{pmatrix} \quad [31]$$

The eigenvalues are 6 and 2, and the eigenvectors are $(1, 0)^{\mathrm{T}}$ and $(0, 1)^{\mathrm{T}}$. Rotation of a reference frame through an angle $-\theta$, which can be visualized as rotating the ellipse through an angle θ, is accomplished by multiplying the tensor by $\mathbf{R}(-\theta)$ on the left and by $\mathbf{R}^{\mathrm{T}}(-\theta)$ on the right:

$$\begin{pmatrix} D'_{xx} & D'_{xy} \\ D'_{yx} & D'_{yy} \end{pmatrix} = \mathbf{R}(-\theta)\mathbf{D}\mathbf{R}^{T}(-\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \times \begin{pmatrix} D_{xx} & D_{xy} \\ D_{xy} & D_{yy} \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \quad [32]$$

The result is

$$D'_{xx} = D_{xx}\cos^2\theta + D_{yy}\sin^2\theta - D_{xy}2\sin\theta\cos\theta \quad [33]$$

$$D'_{xy} = D'_{yx} = D_{xy}(\cos^2\theta - \sin^2\theta) + (D_{xx} - D_{yy})\sin\theta\cos\theta \quad [34]$$

$$D'_{yy} = D_{yy}\cos^2\theta + D_{xx}\sin^2\theta + D_{xy}2\sin\theta\cos\theta \quad [35]$$

The rotation angle required to convert a nondiagonal tensor to a diagonal tensor, θ_{diag}, can be calculated by setting $D'_{xy} = 0$ in Eq. [34]. Remembering that Eqs. [33–35] describe rotation of the reference frame through an angle $-\theta$,

$$D_{xy}\cos 2\theta_{\mathrm{diag}} + [(D_{xx} - D_{yy})/2]\sin 2\theta_{\mathrm{diag}} = 0 \quad [36]$$

$$\tan 2\theta_{\mathrm{diag}} = 2D_{xy}/(D_{yy} - D_{xx}) \quad [37]$$

$$-\theta_{\mathrm{diag}} = \{\arctan[2D_{xy}/(D_{xx} - D_{yy})]\}/2 \quad [38]$$

Thus, rotation of the reference frame through the angle $-\theta_{\mathrm{diag}}$, as defined in Eq. [38], will produce a diagonal tensor. Clearly, the initial nondiagonal tensor had been produced by rotation of the reference frame through the angle $-\theta_{\mathrm{rot}}$, where

$$-\theta_{\mathrm{rot}} = \theta_{\mathrm{diag}} = \{\arctan[2D_{xy}/(D_{yy} - D_{xx})]\}/2 \quad [39]$$

For example, rotating the reference frame of the tensor in Eq. [31] by $-\theta_{\mathrm{rot}} = -30°$, which can be visualized as rotating the ellipse by $\theta_{\mathrm{rot}} = 30°$, produces

$$\begin{pmatrix} 0.866 & -0.5 \\ 0.5 & 0.866 \end{pmatrix}\begin{pmatrix} 6 & 0 \\ 0 & 2 \end{pmatrix}\begin{pmatrix} 0.866 & 0.5 \\ -0.5 & 0.866 \end{pmatrix} = \begin{pmatrix} 5 & 1.732 \\ 1.732 & 3 \end{pmatrix} \quad [40]$$

The calculated rotation angle to produce a diagonal tensor is

$$-\theta_{\mathrm{diag}} = [\arctan(3.464/2)]/2 = 30° \quad [41]$$

The original rotation angle of the reference frame is then calculated to be $-\theta_{\mathrm{rot}} = \theta_{\mathrm{diag}} = -30°$.

Consider what happens when a multiple of the identity matrix, $k\mathbf{I}$, is added to a tensor, $\mathbf{D}$. Each diagonal element increases by the same amount, k, and the off-diagonal elements do not change. This effect remains the same even when the tensor is rotated, because

$$\mathbf{R}(\mathbf{D} + k\mathbf{I})\mathbf{R}^{\mathrm{T}} = \mathbf{R}\mathbf{D}\mathbf{R}^{\mathrm{T}} + k\mathbf{I} \quad [42]$$

Geometrically, this corresponds to changing the length of each ellipsoid axis (which is proportional to the square root of the corresponding eigenvalue) without changing the axis directions (eigenvectors). Because all the eigenvalues change by the same amount, the differences between the eigenvalues to not change.

Rotation of a 2D tensor through any angle has several noteworthy properties:

1. The rotated 2D tensor is symmetric, so the off-diagonal elements are equal.
2. Rotation by $\theta+180°$ is the same as rotation by θ.
3. Rotation by 90° results in the x and y diagonal elements being exchanged, and D_{xy} becomes $-D_{xy}$.
4. The maximum possible value of the off-diagonal element is $(\lambda_1 - \lambda_2)/2$, where $\lambda_1 > \lambda_2$.
5. The off-diagonal element cannot be greater than the smallest diagonal element.

6. For any rotation angle, the diagonal elements range from λ_2 to λ_1, never beyond these limits.
7. For a given pair of eigenvalues, as the magnitude of the off-diagonal element, $|D_{xy}|$, increases, the magnitude of the difference between the two diagonal elements, $|D_{xx} - D_{yy}|$, decreases, and vice versa.

   For positive real eigenvalues, the following properties also apply.
8. The diagonal elements are positive, $D_{xx} > 0$ and $D_{yy} > 0$.
9. The determinant of $\mathbf{D}$ is positive, $\det(\mathbf{D}) > 0$, or $D_{xx}D_{yy} > D_{xy}{}^2$.

Some 2D diffusion ellipses and their associated 2D tensors are shown in Fig. 7.

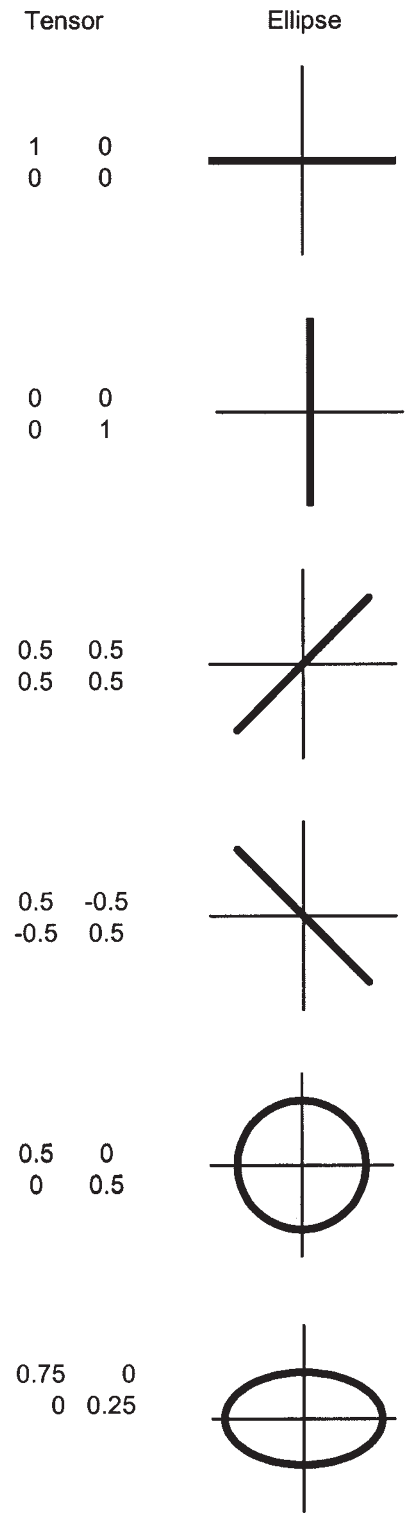

Figure 7 Some examples of 2D tensors and their associated ellipses. The first tensor and the last two tensors were shown in Fig. 1, along with their associated *ADC* "peanuts."

Tensor Rotation in Three Dimensions

The general formula for rotation of a 3D tensor is

$$\begin{pmatrix} D'_{xx} & D'_{xy} & D'_{xz} \\ D'_{xy} & D'_{yy} & D'_{yz} \\ D'_{xz} & D'_{yz} & D'_{zz} \end{pmatrix} = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix} \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix} \times \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \quad [43]$$

The result is

$$D'_{xx} = a^2D_{xx} + d^2D_{yy} + g^2D_{zz} + 2adD_{xy} + 2agD_{xz} + 2dgD_{yz} \quad [44]$$

$$D'_{yy} = b^2D_{xx} + e^2D_{yy} + h^2D_{zz} + 2beD_{xy} + 2bhD_{xz} + 2ehD_{yz} \quad [45]$$

$$D'_{zz} = c^2D_{xx} + f^2D_{yy} + i^2D_{zz} + 2cfD_{xy} + 2ciD_{xz} + 2fiD_{yz} \quad [46]$$

$$D'_{xy} = abD_{xx} + deD_{yy} + ghD_{zz} + (ae + bd)\,D_{xy} + (ah + bg)\,D_{xz} + (dh + eg)\,D_{yz} \quad [47]$$

$$D'_{xz} = acD_{xx} + dfD_{yy} + giD_{zz} + (af + cd)\,D_{xy} + (ai + cg)\,D_{xz} + (di + fg)\,D_{yz} \quad [48]$$

$$D'_{yz} = bcD_{xx} + efD_{yy} + hiD_{zz} + (bf + ce)\,D_{xy} + (bi + ch)\,D_{xz} + (ei + fh)\,D_{yz} \quad [49]$$

For a diagonal tensor $\mathbf{\Lambda}$, this becomes

$$\begin{pmatrix} D'_{xx} & D'_{xy} & D'_{xz} \\ D'_{xy} & D'_{yy} & D'_{yz} \\ D'_{xz} & D'_{yz} & D'_{zz} \end{pmatrix} = \begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix} \begin{pmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_y & 0 \\ 0 & 0 & \lambda_z \end{pmatrix} \times \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \quad [50]$$

where

$$D'_{xx} = a^2\lambda_x + d^2\lambda_y + g^2\lambda_z \quad [51]$$

$$D'_{yy} = b^2\lambda_x + e^2\lambda_y + h^2\lambda_z \quad [52]$$

$$D'_{zz} = c^2\lambda_x + f^2\lambda_y + i^2\lambda_z \quad [53]$$

$$D'_{xy} = ab\lambda_x + de\lambda_y + gh\lambda_z \quad [54]$$

$$D'_{xz} = ac\lambda_x + df\lambda_y + gi\lambda_z \quad [55]$$

$$D'_{yz} = bc\lambda_x + ef\lambda_y + hi\lambda_z \quad [56]$$

Notice that the results of Eqs. [51–56], which apply only to diagonal tensors, do not change when one or more column of the rotation matrix (a, b, and c; or d, e, and f; or g, h, and i) are multiplied by -1. This property is not generally true for rotations of nondiagonal tensors.

Rotation of a 3D tensor through any angle about any axis or combination of axes has the following properties:

1. The rotated tensor is symmetric, $D'_{ij} = D'_{ji}$ for $i \in (x, y, z)$ and $j \in (x, y, z)$.
2. Rotation by $\theta + 180°$ about any ellipsoid axis is the same as rotation by θ.
3. Rotation by 90° about the x, y, or z axis results in the other two diagonal elements (e.g., D_{yy} and D_{zz} for the x axis) being exchanged, and the corresponding off-diagonal element (D_{yz}) being multiplied by -1.
4. The diagonal elements range from $\lambda_{\min}$ to $\lambda_{\max}$, never beyond these limits.
   For positive real eigenvalues, the following properties also apply.
5. The diagonal elements are positive: $D_{xx} > 0$, $D_{yy} > 0$, and $D_{zz} > 0$.
6. The determinant of $\mathbf{D}$ is positive, $\det(\mathbf{D}) > 0$.
7. For all i and j, $D_{ii} + D_{jj} > 2D_{ij}$.
8. The off-diagonal elements are all smaller than the largest diagonal element.

The same rotation matrices that were derived for vector rotations can be applied to tensor rotations. This includes rotations by specific angles about specified axes, and rotations so that vectors initially along the x, y, and z axes end up in specified other positions. If the original tensor is diagonal, then the columns of the rotation matrix are the three eigenvectors of the rotated tensor.

In computer simulations it is common to begin with a diagonal tensor whose diagonal elements are the eigenvalues, representing a diffusion ellipsoid aligned with the gradient x, y, z reference frame:

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_y & 0 \\ 0 & 0 & \lambda_z \end{pmatrix} \quad [57]$$

This ellipsoid is then rotated to a desired orientation, or to random orientations. Typically the ellipsoid is rotated about its longest axis by an angle Ψ, then the long axis is rotated to a desired orientation with respect to the x, y, and z axes. If the longest axis is initially along the z axis, the resulting rotation matrix can be represented as

$$\mathbf{R} = \mathbf{R}(z, -\phi)\mathbf{R}(y, -\theta)\mathbf{R}(z, -\psi) \quad [58]$$

$$\mathbf{R} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \times \begin{pmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad [59]$$

and the resulting tensor is given by

$$\mathbf{D} = \mathbf{R}\Lambda\mathbf{R}^{\mathrm{T}} = \mathbf{R}(z, -\phi)\mathbf{R}(y, -\theta)\mathbf{R}(z, -\psi) \times \Lambda\mathbf{R}(z, \psi)\mathbf{R}(y, \theta)\mathbf{R}(z, \phi) \quad [60]$$

where the individual rotation matrices are shown in Eqs. [16–18]. The final result is identical to published rotation formulas, which reversed the definitions and positions of $\mathbf{R}$ and $\mathbf{R}^{\mathrm{T}}$ (*40*, *43*).

Rotational Invariants

Several properties of the diffusion tensor are rotationally invariant (they do not change when the tensor is rotated through any angle θ). Therefore, these properties can be calculated for any tensor orientation, without tensor diagonalization. Many of these rotational invariants are useful in deriving quantitative information from the diffusion tensor, including the mean diffusivity and several measurements of anisotropy, and in comparing different tensors and ellip-

Table 1 Rotationally Invariant Parameters of 3D Diffusion Tensors Expressed in Terms of Eigenvalues

Parameter	Synonyms	Eigenvalue Formula
I_1	Trace	$\lambda_1 + \lambda_2 + \lambda_3$
I_2		$\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1$
I_3	Determinant	$\lambda_1\lambda_2\lambda_3$
I_4	$I_1^2 - 2I_2 = \mathbf{D}{:}\mathbf{D} = \mathrm{Trace}(\mathbf{D}^2)$	$\lambda_1^2 + \lambda_2^2 + \lambda_3^2$
D_{av}	$I_1/3$; "A"	$(\lambda_1 + \lambda_2 + \lambda_3)/3$
D_{surf}	$(I_2/3)^{1/2}$; "J"	$[(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1)/3]^{1/2}$
D_{vol}	$I_3^{1/3}$; "G"	$(\lambda_1\lambda_2\lambda_3)^{1/3}$
D_{mag}	$(I_4/3)^{1/2} = (3D_{\mathrm{av}}^2 - 2D_{\mathrm{surf}}^2)^{1/2}$	$[(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)/3]^{1/2}$
$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$	$6D_{\mathrm{av}}^2 - 2I_2$	$(\lambda_1 - D_{\mathrm{av}})^2 + (\lambda_2 - \mathrm{D}_{\mathrm{av}})^2 + (\lambda_3 - D_{\mathrm{av}})^2$
"K"	I_2/I_1	$(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1)/D_{\mathrm{av}}$
"H"	$3I_3/I_2$	$3\lambda_1\lambda_2\lambda_3/(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1)$

Note: $\mathbf{D}_{\mathrm{an}}$ is the anisotropic part of $\mathbf{D}$ (Eq. [67]).

soids. These properties therefore deserve further discussion here.

The 3D invariants are expressed in terms of the eigenvectors in Table 1, and in terms of the tensor elements in Table 2. The 2D invariants are expressed in terms of the eigenvectors in Table 3, and in terms of the tensor elements in Table 4. Some of these invariants, which include the trace (the sum of the diagonal elements) and the determinant, are useful in calculating eigenvalues and eigenvectors, and in defining anisotropy indices. The three invariants I_1, I_2, and I_3 have been called the "scalar invariants" (*4*) and the "principal invariants" (*44*, *45*), and have also been named J_1, J_2, and J_3 (*46*). They have been defined in terms of the eigenvalues (*4*, *44*, *47*) and in terms of the tensor elements (*18*, *44*, *46*, *48*).

Other invariants can be expressed in terms of these three scalar or principal invariants. For example, the tensor dot product is analogous to the vector dot product:

$$\mathbf{D}{:}\mathbf{D} = \sum_{i=1}^{3}\sum_{j=1}^{3} D_{ij}^2 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \quad [61]$$

$$\mathbf{D}{:}\mathbf{D} = D_{xx}^2 + D_{yy}^2 + D_{zz}^2 + 2(D_{xy}^2 + D_{xz}^2 + D_{yz}^2) \quad [62]$$

$\mathbf{D}{:}\mathbf{D}$ is often considered another scalar or principal invariant, I_4 (or I_3 in 2D), although it can be expressed in terms of I_1 and I_2 (*45*, *48*, *49*):

$$\mathbf{D}{:}\mathbf{D} = I_4 = I_1^2 - 2I_2 \quad [63]$$

$$\mathbf{D}{:}\mathbf{D} = I_3 = I_1^2 - 2I_2 \quad (2\mathrm{D}) \quad [64]$$

$\mathbf{D}{:}\mathbf{D}$ can also be expressed in terms of $\mathbf{D}^2$:

$$\mathbf{D}^2 = \mathbf{DD} = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}\begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix} \quad [65]$$

Table 2 Rotationally Invariant Parameters of 3D Diffusion Tensors Expressed in Terms of Tensor Elements

Parameter	Tensor Element Formula
I_1	$D_{xx} + D_{yy} + D_{zz}$
I_2	$D_{xx}D_{yy} + D_{yy}D_{zz} + D_{zz}D_{xx} - (D_{xy}^2 + D_{xz}^2 + D_{yz}^2)$
I_3	$D_{xx}D_{yy}D_{zz} + 2D_{xy}D_{xz}D_{yz} - (D_{zz}D_{xy}^2 + D_{yy}D_{xz}^2 + D_{xx}D_{yz}^2)$
I_4	$D_{xx}^2 + D_{yy}^2 + D_{zz}^2 + 2(D_{xy}^2 + D_{xz}^2 + D_{yz}^2)$
D_{av}	$(D_{xx} + D_{yy} + D_{zz})/3$
D_{surf}	$\{[D_{xx}D_{yy} + D_{yy}D_{zz} + D_{zz}D_{xx} - (D_{xy}^2 + D_{xz}^2 + D_{yz}^2)]/3\}^{1/2}$
D_{vol}	$[D_{xx}D_{yy}D_{zz} + 2D_{xy}D_{xz}D_{yz} - (D_{zz}D_{xy}^2 + D_{yy}D_{xz}^2 + D_{xx}D_{yz}^2)]^{1/3}$
D_{mag}	$\{[D_{xx}^2 + D_{yy}^2 + D_{zz}^2 + 2(D_{xy}^2 + D_{xz}^2 + D_{yz}^2)]/3\}^{1/2}$
$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$	$(D_{xx} - D_{\mathrm{av}})^2 + (D_{yy} - D_{\mathrm{av}})^2 + (D_{zz} - D_{\mathrm{av}})^2 + 2D_{xy}^2 + 2D_{xz}^2 + 2D_{yz}^2$
"K"	$[(D_{xx}D_{yy} + D_{yy}D_{zz} + D_{zz}D_{xx}) - (D_{xy}^2 + D_{xz}^2 + D_{yz}^2)]/(D_{xx} + D_{yy} + D_{zz})$
"H"	$3[D_{xx}D_{yy}D_{zz} + 2D_{xy}D_{xz}D_{yz} - (D_{zz}D_{xy}^2 + D_{yy}D_{xz}^2 + D_{xx}D_{yz}^2)]/[(D_{xx}D_{yy} + D_{yy}D_{zz} + D_{zz}D_{xx}) - (D_{xy}^2 + D_{xz}^2 + D_{yz}^2)]$

Note: $\mathbf{D}_{\mathrm{an}}$ is the anisotropic part of $\mathbf{D}$ (Eq. [67]).

Table 3 Rotationally Invariant Parameters of 2D Diffusion Tensors Expressed in Terms of Eigenvalues

Index	Synonyms	Eigenvalue Formula
I_1	Trace	$\lambda_1 + \lambda_2$
I_2	Determinant	$\lambda_1\lambda_2$
I_3	$I_1^2 - 2I_2 = \mathbf{D}{:}\mathbf{D} = \mathrm{Trace}(\mathbf{D}^2)$	$\lambda_1^2 + \lambda_2^2$
D_{av}	$I_1/2 =$ "A"	$(\lambda_1 + \lambda_2)/2$
D_{area}	$I_2^{1/2} =$ "J", "G"	$(\lambda_1\lambda_2)^{1/2}$
D_{mag}	$(I_3/2)^{1/2} = (2D_{\mathrm{av}}^2 - D_{\mathrm{area}}^2)^{1/2}$	$[(\lambda_1^2 + \lambda_2^2)/2]^{1/2}$
$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$		$(\lambda_1 - D_{\mathrm{av}})^2 + (\lambda_2 - D_{\mathrm{av}})^2$
H, K	$2I_2/I_1$	$2\lambda_1\lambda_2/(\lambda_1 + \lambda_2)$

Note: $\mathbf{D}_{\mathrm{an}}$ is the anisotropic part of $\mathbf{D}$ (Eq. [67]).

$$\mathbf{D}{:}\mathbf{D} = \mathrm{Trace}(\mathbf{D}^2) \qquad [66]$$

When the isotropic part of the tensor, $D_{\mathrm{av}}\,\mathbf{I}$, is subtracted from the whole tensor, $\mathbf{D}$, the remainder is considered to be the anisotropic part of the tensor. The anisotropic part of $\mathbf{D}$ has been indicated by italics, $\boldsymbol{D}$, which can lead to confusion when formulas are incorrectly typeset (*50*), and by the letter A (*51*), which could be confused with the cylindrical symmetry anisotropy index A, which will be defined in Part II. An alternative is the notation $\mathbf{D}_{\mathrm{an}}$ (*44*), so that

$$\mathbf{D}_{\mathrm{an}} = \mathbf{D} - D_{\mathrm{av}}\mathbf{I} \qquad [67]$$

$$\mathbf{D}_{\mathrm{an}} = \begin{pmatrix} D_{xx} - D_{\mathrm{av}} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} - D_{\mathrm{av}} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} - D_{\mathrm{av}} \end{pmatrix} \qquad [68]$$

The discussion around Eq. [42] shows that $\mathbf{D}$ and $\mathbf{D}_{\mathrm{an}}$ have the same eigenvectors, and this has also been shown by Basser and Pierpaoli (*52*). In addition, the tensor dot product of $\mathbf{D}_{\mathrm{an}}$, $\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$, is rotationally invariant (*52*). It can be shown (*50*) that in 3D,

$$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}} = \mathbf{D}{:}\mathbf{D} - 3D_{\mathrm{av}}^2 = \mathbf{D}{:}\mathbf{D} - I_1^2/3 \qquad [69]$$

$$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}} = 6D_{\mathrm{av}}^2 - 2I_2 \qquad [70]$$

$$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}} = (2/3)(D_{xx}^2 + D_{yy}^2 + D_{zz}^2 - D_{xx}D_{yy} - D_{xx}D_{zz} - D_{yy}D_{zz}) + 2(D_{xy}^2 + D_{xz}^2 + D_{yz}^2) \qquad [71]$$

Eq. [70] follows from Eqs. [63] and [69] and the definition of I_1. $\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$ may be considered to be proportional to the variance of the eigenvalues in 3D or 2D (*52*):

$$\sigma_\lambda^2 = \mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}/3 = [(\lambda_1 - \lambda_{\mathrm{av}})^2 + (\lambda_2 - \lambda_{\mathrm{av}})^2 + (\lambda_3 - \lambda_{\mathrm{av}})^2]/3 \qquad [72]$$

$$\sigma_\lambda^2 = \mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}/2 = [(\lambda_1 - \lambda_{\mathrm{av}})^2 + (\lambda_2 - \lambda_{\mathrm{av}})^2]/2 \quad \text{(2D)} \qquad [73]$$

Tensor dot products can be calculated between two different tensors, similar to the vector dot product. These are also rotationally invariant, in the sense that the result does not change if the same rotation is applied to both tensors:

$$\mathbf{D}{:}\mathbf{D}' = D_{xx}D'_{xx} + D_{yy}D'_{yy} + D_{zz}D'_{zz} + 2(D_{xy}D'_{xy} + D_{xz}D'_{xz} + D_{yz}D'_{yz}) \qquad [74]$$

$$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}'_{\mathrm{an}} = (D_{xx} - D_{\mathrm{av}})(D'_{xx} - D'_{\mathrm{av}}) + (D_{yy} - D_{\mathrm{av}})(D'_{yy} - D'_{\mathrm{av}}) + (D_{zz} - D_{\mathrm{av}})(D'_{zz} - D'_{\mathrm{av}}) + 2(D_{xy}D'_{xy} + D_{xz}D'_{xz} + D_{yz}D'_{yz}) \qquad [75]$$

Several formulas involving rotational invariants have been published, including Eqs. [76] (*13*, *50*) and [77] (*18*).

$$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}'_{\mathrm{an}} = \mathbf{D}{:}\mathbf{D}' - 3D_{\mathrm{av}}D'_{\mathrm{av}} = \mathbf{D}{:}\mathbf{D}' - I_1I'_1/3 \qquad [76]$$

Table 4 Rotationally Invariant Parameters of 2D Diffusion Tensors Expressed in Terms of Tensor Elements

Index	Tensor Element Formula
I_1	$D_{xx} + D_{yy}$
I_2	$D_{xx}D_{yy} - D_{xy}^2$
I_3	$D_{xx}^2 + D_{yy}^2 + 2D_{xy}^2$
D_{av}	$(D_{xx} + D_{yy})/2$
D_{area}	$(D_{xx}D_{yy} - D_{xy}^2)^{1/2}$
D_{mag}	$[(D_{xx}^2 + D_{yy}^2 + 2D_{xy}^2)/2]^{1/2}$
$\mathbf{D}_{\mathrm{an}}{:}\mathbf{D}_{\mathrm{an}}$	$(D_{xx} - D_{\mathrm{av}})^2 + (D_{yy} - D_{\mathrm{av}})^2 + 2D_{xy}^2$
H, K	$2(D_{xx}D_{yy} - D_{xy}^2)/(D_{xx} + D_{yy})$

Note: $\mathbf{D}_{\mathrm{an}}$ is the anisotropic part of $\mathbf{D}$ (Eq. [67]).

$$I_2 = [\mathrm{Trace}^2(\mathbf{D}) - \mathrm{Trace}(\mathbf{D}^2)]/2 \qquad [77]$$

Ulug and van Zijl defined D_{av}, D_{surf}, D_{vol}, and D_{mag} in terms of I_1, I_2, I_3, and I_4, scaled and modified to have the same units as diffusion coefficients (length^2/time) (*48*). Bahn used single letters of the alphabet to define A (arithmetic mean $= D_{av}$), G (geometric mean $= D_{vol}$), H (harmonic mean), J (D_{surf}), and K, and stated that $A > J > G$ ($D_{av} > D_{surf} > D_{vol}$) (*47*). Presumably the names J and K were chosen because they follow I in the alphabet. (These names should not be confused with two functions that will be discussed in Part II: The Heaviside Unit-Step Function, H, and the cylindrical symmetry anisotropy index, A.)

Important Points in "Tensors and Tensor Rotations"

The rotation matrices that were derived for vectors can be applied to tensors, but it is also necessary to multiply on the right by the transpose (which is the inverse) of the rotation matrix (Eqs. [27], [32], [43], [50], and [60]). As with vectors, rotations can be specified as a rotation through a specified angle about a specified axis, or a rotation to a desired final position for vectors initially along the x, y, and z axes. The expanded results of tensor (matrix) rotation are shown in Eqs. [27–30] (2D) and Eqs. [43–56] (3D). Some of the rotationally invariant properties of a tensor are shown in Tables 1–4.

CALCULATION OF EIGENVECTORS AND EIGENVALUES

The purposes of this section are to explain 1) the meaning of the eigenvectors and eigenvalues of the diffusion tensor, 2) how the eigenvectors and eigenvalues can be calculated analytically, and 3) that they represent the directions of the principal axes of the diffusion ellipsoid and the squares of the hemiaxis lengths, respectively. This allows the size, shape, and orientation of the diffusion ellipsoid to be calculated directly from the diffusion tensor.

General Eigenvector Equations

Consider a diffusion ellipsoid perfectly aligned with the gradient reference frame, so that its tensor is diagonal (Eq. [57]). The diagonal elements λ_1, λ_2, and λ_3 are called eigenvalues. The root mean squared displacement along each of the three principle axes of the ellipsoid is proportional to $(2\lambda_i t)^{1/2}$, where t is the diffusion time. The unit vectors that point along the ellipsoid axes—$(1, 0, 0)^T$, $(0, 1, 0)^T$, and $(0, 0, 1)^T$—are called eigenvectors. Each eigenvector corresponds to one eigenvalue. When the ellipsoid is rotated, the tensor has the same eigenvalues and different eigenvectors. The eigenvalues and eigenvectors usually are not immediately obvious from the tensor. Eigenvectors and eigenvalues are related by the fact that when the tensor is multiplied by an eigenvector, the result is the same eigenvector multiplied by the eigenvalue:

$$\mathbf{D}\varepsilon_i = \lambda_i\varepsilon_i = \lambda_i\mathbf{I}\varepsilon_i \quad i = \{1, 2, 3\} \qquad [78]$$

$$\begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}\begin{pmatrix} \varepsilon_{ix} \\ \varepsilon_{iy} \\ \varepsilon_{iz} \end{pmatrix} = \lambda_i\begin{pmatrix} \varepsilon_{ix} \\ \varepsilon_{iy} \\ \varepsilon_{iz} \end{pmatrix} \qquad [79]$$

This is matrix notation for the following equations:

$$D_{xx}\varepsilon_{ix} + D_{xy}\varepsilon_{iy} + D_{xz}\varepsilon_{iz} = \lambda_i\varepsilon_{ix} \qquad [80]$$

$$D_{xy}\varepsilon_{ix} + D_{yy}\varepsilon_{iy} + D_{yz}\varepsilon_{iz} = \lambda_i\varepsilon_{iy} \qquad [81]$$

$$D_{xz}\varepsilon_{ix} + D_{yz}\varepsilon_{iy} + D_{zz}\varepsilon_{iz} = \lambda_i\varepsilon_{iz} \qquad [82]$$

Equation [78] can be rewritten in matrix form as

$$\mathbf{DE} = \mathbf{E}\Lambda \qquad [83]$$

$$\begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}\begin{pmatrix} \varepsilon_{1x} & \varepsilon_{2x} & \varepsilon_{3x} \\ \varepsilon_{1y} & \varepsilon_{2y} & \varepsilon_{3y} \\ \varepsilon_{1z} & \varepsilon_{2z} & \varepsilon_{3z} \end{pmatrix} = \begin{pmatrix} \varepsilon_{1x} & \varepsilon_{2x} & \varepsilon_{3x} \\ \varepsilon_{1y} & \varepsilon_{2y} & \varepsilon_{3y} \\ \varepsilon_{1z} & \varepsilon_{2z} & \varepsilon_{3z} \end{pmatrix} \times \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \qquad [84]$$

where $\mathbf{E}$, the eigenvector matrix, is produced by writing the orthonormal eigenvectors as column vectors, and $\mathbf{\Lambda}$ is the eigenvalue matrix (Eq. [57]) (*4*, *52*). Because the three eigenvectors are orthonormal, $\mathbf{E}$ has the properties of a rotation matrix, including

$$\mathbf{E}^{-1} = \mathbf{E}^{T} \qquad [85]$$

Equation [83] can therefore be used to calculate $\mathbf{D}$ from $\mathbf{\Lambda}$, or $\mathbf{\Lambda}$ from $\mathbf{D}$:

$$\mathbf{DEE}^{T} = \mathbf{D} = \mathbf{E}\Lambda\mathbf{E}^{T} \qquad [86]$$

$$\mathbf{E}^{T}\mathbf{E}\Lambda = \Lambda = \mathbf{E}^{T}\mathbf{DE} \qquad [87]$$

Equation [86] shows how to produce a tensor with any desired eigenvectors from a diagonal tensor with specified eigenvalues. Comparison with Eqs. [32] and [60] shows that the reference frame is rotated in the direction away from the eigenvectors, which can be visualized as the tensor (ellipse) rotating to the eigenvector positions. Equation [87] shows how to reverse this process and produce a diagonal tensor (the eigenvalue matrix) by using the eigenvector matrix to perform the opposite rotation, rotating the reference frame to the eigenvector position so that the eigenvectors are aligned with the axes of the reference frame.

The eigenvalues and eigenvectors can be calculated by application of Eq. [78]. Subtracting $\lambda_i \mathbf{I} \varepsilon_i$ from each side yields

$$(\mathbf{D} - \lambda_i \mathbf{I})\varepsilon_i = 0 \qquad [88]$$

$$\begin{pmatrix} D_{xx} - \lambda_i & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} - \lambda_i & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} - \lambda_i \end{pmatrix} \begin{pmatrix} \varepsilon_{ix} \\ \varepsilon_{iy} \\ \varepsilon_{iz} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad [89]$$

This is matrix notation for the following equations:

$$(D_{xx} - \lambda_i)\varepsilon_{ix} + D_{xy}\varepsilon_{iy} + D_{xz}\varepsilon_{iz} = 0 \qquad [90]$$

$$D_{xy}\varepsilon_{ix} + (D_{yy} - \lambda_i)\varepsilon_{iy} + D_{yz}\varepsilon_{iz} = 0 \qquad [91]$$

$$D_{xz}\varepsilon_{ix} + D_{yz}\varepsilon_{iy} + (D_{zz} - \lambda_i)\varepsilon_{iz} = 0 \qquad [92]$$

A set of homogeneous equations like this has a nontrivial solution only if the determinant of $(\mathbf{D} - \lambda_i \mathbf{I})$ is zero:

$$\det(\mathbf{D} - \lambda_i \mathbf{I}) = 0 \qquad [93]$$

This results in an n-th order polynomial equation where n is the matrix dimension. For example, in 2D, Eq. [93] corresponds to

$$(D_{xx} - \lambda_i)(D_{yy} - \lambda_i) - D_{xy}^2 = 0 \quad \text{(2D)} \qquad [94]$$

and in 3D Eq. [93] corresponds to

$$\begin{aligned}(D_{xx} - \lambda_i)&[(D_{yy} - \lambda_i)(D_{zz} - \lambda_i) - D_{yz}^2] \\ &- D_{xy}[D_{xy}(D_{zz} - \lambda_i) - D_{xz}D_{yz}] \\ &+ D_{xz}[D_{xy}D_{yz} - D_{xz}(D_{yy} - \lambda_i)] = 0 \qquad [95]\end{aligned}$$

In the general n-dimensional case, a number of methods are available for estimating the eigenvalues (*53*). The analytic solutions for the 2D quadratic equation and the 3D cubic equation are discussed in the next two sections.

2D Eigenvalues and Eigenvectors

In the 2D case, Eq. [94] can be written as

$$\lambda^2 - I_1\lambda + I_2 = 0 \qquad [96]$$

where I_1 and I_2 are two rotationally invariant parameters, the trace and the determinant of the tensor (see Tables 3 and 4). This quadratic equation is easily solved with the quadratic formula, yielding

$$\lambda_1 = [I_1 + (I_1^2 - 4I_2)^{1/2}]/2 \qquad [97]$$

$$\begin{aligned}\lambda_1 = \{D_{xx} + D_{yy} + [&(D_{xx} + D_{yy})^2 \\ &- 4(D_{xx}D_{yy} - D_{xy}^2)]^{1/2}\}/2 \qquad [98]\end{aligned}$$

$$\lambda_2 = [I_1 - (I_1^2 - 4I_2)^{1/2}]/2 \qquad [99]$$

$$\begin{aligned}\lambda_2 = \{D_{xx} + D_{yy} - [&(D_{xx} + D_{yy})^2 \\ &- 4(D_{xx}D_{yy} - D_{xy}^2)]^{1/2}\}/2 \qquad [100]\end{aligned}$$

The eigenvectors can be determined by applying Eq. [88] to each eigenvalue. For each eigenvalue this provides two equations in two unknowns:

$$(D_{xx} - \lambda_i)\varepsilon_x + D_{xy}\varepsilon_y = 0 \qquad [101]$$

$$D_{xy}\varepsilon_x + (D_{yy} - \lambda_i)\varepsilon_y = 0 \qquad [102]$$

However, these two equations are not independent. There is not a unique solution because the determinant in Eq. [93] is zero. This occurs because the length of an eigenvector is not specified, only its direction and therefore the ratio $\varepsilon_y/\varepsilon_x$. The ratio $\varepsilon_y/\varepsilon_x$ can be determined from either Eq. [101] or [102]:

$$\varepsilon_y/\varepsilon_x = -(D_{xx} - \lambda_i)/D_{xy} \qquad [103]$$

$$\varepsilon_y/\varepsilon_x = -D_{xy}/(D_{yy} - \lambda_i) \qquad [104]$$

The ratios in Eqs. [103] and [104] are equal because of Eq. [94]. One normalized eigenvector can then be calculated from Eq. [103] as

$$\varepsilon_1 = [1, -(D_{xx} - \lambda_1)/D_{xy}]/M_2 \qquad [105]$$

where the magnitude of the unnormalized vector is

$$M_2 = [1 + (D_{xx} - \lambda_1)^2/D_{xy}^2]^{1/2} \qquad [106]$$

If $D_{xy} = 0$, then the tensor was already diagonal, and the diagonal elements are the eigenvalues. The other eigenvector can be calculated the same way from Eq.

[104]. However, since the two eigenvectors must be orthogonal,

$$\varepsilon_2 = [(D_{xx} - \lambda_1)/D_{xy}, 1]/M_2 \quad [107]$$

Keep in mind that the negative of each eigenvector is also an eigenvector with the same eigenvalue. Thus, $-\varepsilon_1$ and $-\varepsilon_2$ are also valid eigenvectors.

If the tensor $\mathbf{D}$ is already diagonal, this eigenvector solution fails because of division by 0 in Eq. [103]. In this case the eigenvectors are along the x and y axis. If the two eigenvalues are equal (degenerate), the tensor is always diagonal, and the eigenvectors are not uniquely defined. A diagonal tensor is unlikely to arise with actual data, but could arise in computer simulations with no noise.

In applying Eq. [87] to produce a diagonal tensor, the result is not changed by replacing ε_1 by $-\varepsilon_1$ or ε_2 by $-\varepsilon_2$. That is, one or more columns of $\mathbf{E}$ (and the corresponding rows of $\mathbf{E}^T$) can be multiplied by -1 without changing the results of Eqs. [86] and [87]. This is an example of the property mentioned after Eq. [56]. Therefore, two distinct eigenvector matrices can be formed, $[\pm\varepsilon_1, \pm\varepsilon_2]$ and $[\pm\varepsilon_2, \pm\varepsilon_1]$. In the diagonal tensor resulting from application of Eq. [87], the eigenvalue corresponding to the first eigenvector will appear as D_{xx}, and the eigenvalue corresponding to the second eigenvector will appear as D_{yy}.

3D Eigenvalues and Eigenvectors

In the 3D case,

$$\lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 = 0 \quad [108]$$

where the rotational invariants I_1, I_2, and I_3 are defined in Tables 1 and 2. The solution to this cubic equation is more complex than the 2D solution (*53*) but still manageable (*44*). The sorted eigenvalues ($\lambda_1 > \lambda_2 > \lambda_3$) are

$$\lambda_1 = I_1/3 + 2v^{1/2}\cos(\phi) \quad [109]$$

$$\lambda_2 = I_1/3 - 2v^{1/2}\cos(\pi/3 + \phi) \quad [110]$$

$$\lambda_3 = I_1/3 - 2v^{1/2}\cos(\pi/3 - \phi) \quad [111]$$

where

$$v = (I_1/3)^2 - I_2/3 = \mathbf{D}_{an}:\mathbf{D}_{an}/6 \quad [112]$$

$$s = (I_1/3)^3 - I_1I_2/6 + I_3/2 \quad [113]$$

$$\phi = \arccos[s/v^{3/2}]/3 \quad [114]$$

The third eigenvalue can also be calculated from $\lambda_3 = I_1 - \lambda_1 - \lambda_2$ (*44*).

The eigenvectors can be determined, as in the 2D case, by applying Eqs. [90–92] to determine any two of the three ratios $\varepsilon_{iy}/\varepsilon_{ix}$, $\varepsilon_{iz}/\varepsilon_{iy}$, and $\varepsilon_{ix}/\varepsilon_{iz}$. Following the notation of (*44*), the diagonal elements of $\mathbf{D} - \lambda_i \mathbf{I}$ are defined as

$$A_i = D_{xx} - \lambda_i; \quad B_i = D_{yy} - \lambda_i; \quad C_i = D_{zz} - \lambda_i \quad [115]$$

After setting ε_{iz} to an arbitrary value in Eqs. [90] and [91],

$$A_i\varepsilon_{ix} + D_{xy}\varepsilon_{iy} = -D_{xz}\varepsilon_{iz} \quad [116]$$

$$D_{xy}\varepsilon_{ix} + B_i\varepsilon_{iy} = -D_{yz}\varepsilon_{iz} \quad [117]$$

Solution of these two equations yields

$$\varepsilon_{ix} = \varepsilon_{iz}(D_{xy}D_{yz} - B_iD_{xz})/(A_iB_i - D_{xy}^2) \quad [118]$$

$$\varepsilon_{iy} = \varepsilon_{iz}(D_{xy}D_{xz} - A_iD_{yz})/(A_iB_i - D_{xy}^2) \quad [119]$$

$$\varepsilon_{ix}/\varepsilon_{iy} = (D_{xy}D_{yz} - B_iD_{xz})/(D_{xy}D_{xz} - A_iD_{yz}) \quad [120]$$

Similar calculations setting ε_{iy} or ε_{ix} to an arbitrary value yield

$$\varepsilon_{iy}/\varepsilon_{iz} = (D_{xz}D_{yz} - C_iD_{xy})/(D_{xy}D_{yz} - B_iD_{xz}) \quad [121]$$

$$\varepsilon_{iz}/\varepsilon_{ix} = (D_{xy}D_{xz} - A_iD_{yz})/(D_{xz}D_{yz} - C_iD_{xy}) \quad [122]$$

The ratios in Eqs. [120–122] are satisfied by setting

$$\varepsilon_{ix} = (D_{xy}D_{yz} - B_iD_{xz})(D_{xz}D_{yz} - C_iD_{xy}) \quad [123]$$

$$\varepsilon_{iy} = (D_{xz}D_{yz} - C_iD_{xy})(D_{xy}D_{xz} - A_iD_{yz}) \quad [124]$$

$$\varepsilon_{iz} = (D_{xy}D_{xz} - A_iD_{yz})(D_{xy}D_{yz} - B_iD_{xz}) \quad [125]$$

The normalized eigenvectors can be calculated by dividing by the magnitude of the eigenvector,

$$\hat{\boldsymbol{\varepsilon}}_i = \boldsymbol{\varepsilon}_i/\sqrt{\boldsymbol{\varepsilon}_i^T\boldsymbol{\varepsilon}_i} = \boldsymbol{\varepsilon}_i/\sqrt{\varepsilon_{ix}^2 + \varepsilon_{iy}^2 + \varepsilon_{iz}^2} \quad [126]$$

This procedure can be repeated for each eigenvalue. The third eigenvector can also be calculated from the cross product of the first two eigenvectors,

$$\hat{\boldsymbol{\varepsilon}}_3 = \hat{\boldsymbol{\varepsilon}}_1 \times \hat{\boldsymbol{\varepsilon}}_2 = [\varepsilon_{1y}\varepsilon_{2z} - \varepsilon_{2y}\varepsilon_{1z}, \varepsilon_{1z}\varepsilon_{2x} - \varepsilon_{2z}\varepsilon_{1x}, \varepsilon_{1x}\varepsilon_{2y} - \varepsilon_{2x}\varepsilon_{1y}]^{\mathrm{T}} \quad [127]$$

As in the 2D case, this eigenvector solution fails if **D** is diagonal. In this case the eigenvectors are along the x, y, and z axes. A diagonal tensor is unlikely to arise with actual data, but could arise in simulations with no noise.

As in the 2D case, in applying Eq. [87] to produce a diagonal tensor, the result is not changed by replacing ε_1 by $-\varepsilon_1$, ε_2 by $-\varepsilon_2$, or ε_3 by $-\varepsilon_3$. Therefore, six distinct eigenvector matrices can be formed. In the diagonal tensor resulting from application of Eq. [87], the eigenvalue corresponding to the first eigenvector will appear as D_{xx}, the eigenvalue corresponding to the second eigenvector will appear as D_{yy}, and the eigenvalue corresponding to the third eigenvector will appear as D_{zz}. If two or three eigenvalues are equal (degenerate), there is not a unique eigenvector solution. Any linear combination of the two degenerate eigenvectors is also an eigenvector.

Dyadic Tensors

The dyadic tensor was introduced in Eq. [4]. The dyadic tensor produced from an eigenvector is given by

$$\boldsymbol{\varepsilon}_i\boldsymbol{\varepsilon}_i^T = \begin{pmatrix} \varepsilon_{ix} \\ \varepsilon_{iy} \\ \varepsilon_{iz} \end{pmatrix} (\varepsilon_{ix} \quad \varepsilon_{iy} \quad \varepsilon_{iz}) = \begin{pmatrix} \varepsilon_{ix}^2 & \varepsilon_{ix}\varepsilon_{iy} & \varepsilon_{ix}\varepsilon_{iz} \\ \varepsilon_{ix}\varepsilon_{iy} & \varepsilon_{iy}^2 & \varepsilon_{iy}\varepsilon_{iz} \\ \varepsilon_{ix}\varepsilon_{iz} & \varepsilon_{iy}\varepsilon_{iz} & \varepsilon_{iz}^2 \end{pmatrix} \quad [128]$$

An excellent summary of the properties of dyadic tensors produced from the eigenvectors has been given (*41*). These dyadic tensors have been used for two purposes. First, dyadic tensors are useful when eigenvectors must be averaged for data analysis (*41*, *54*). Because the sign of the eigenvector is indeterminate, summation of eigenvectors may result in partial cancellation. In contrast, the dyadic tensors formed from ε_i and $-\varepsilon_i$ are identical, so summation of the dyadic tensors does not have this same problem. The averaged eigenvector can be recovered by calculating the largest eigenvector of the averaged dyadic tensor (*41*). Second, dyadic tensors can be used for sorting eigenvalues, to decrease the noise-induced bias of eigenvalues that are close together relative to the noise level (*41*).

The diffusion tensor can be expressed in terms of the three dyadic tensors formed from the three eigenvalues (*41*):

$$\mathbf{D} = \lambda_1\varepsilon_1\varepsilon_1^{\mathrm{T}} + \lambda_2\varepsilon_2\varepsilon_2^{\mathrm{T}} + \lambda_3\varepsilon_3\varepsilon_3^{\mathrm{T}} \quad [129]$$

Important Points in "Calculation of Eigenvectors and Eigenvalues"

The eigenvectors and eigenvalues of the diffusion tensor represent the directions of the principal axes of the diffusion ellipsoid and the squares of the hemiaxis lengths, respectively. Equation [83] shows the fundamental eigenvalue and eigenvector equation in matrix form. Equations [86] and [87] show how to rotate a diagonal tensor so that it has specified eigenvectors, and how to rotate a nondiagonal tensor to produce a diagonal tensor. Eigenvalues and eigenvectors of 2D tensors (Eqs. [97–100] and [105–107]) and 3D tensors (Eqs. [109–115] and [123–127]) can be determined analytically. Dyadic tensors formed from the eigenvectors can be useful when comparing or averaging multiple tensors.

APPENDIX

The mistakes presented here are primarily typographical and mathematical, not conceptual, errors. Although some of the mistakes listed here are discussed in parts II and III, they are included here so that the following list will be more comprehensive.

Incorrect Formulas Whose Correct Versions Are Shown in Part I

In (*18*), the I_3 part of Eq. [13] should have the product of the eigenvalues, not their sum. In Eq. [15], the last term should be $3\langle\lambda\rangle$, not $\langle\lambda\rangle$.

Incorrect Formulas Whose Correct Versions Will Be Shown in Part II

In (*5*), the definition of fractional anisotropy (FA) (Eq. [30]) is incorrect. (Also, in Eq. [5], $\mathbf{r}^{\mathrm{T}}\mathbf{r}$ should be $-\mathbf{r}^{\mathrm{T}}\mathbf{r}$.)

In (*50*), the definition of LI_N in Eq. [5] is incorrect. The published erratum did not include italics or boldface letters. On page 903, line 8, Table 2 should be Table 4.

In (*55*), in Eq. [7], K_D should be κ_D.

In (*26*), above Fig. 5, $\gamma^2 g^2 \Delta^2(\Delta - \delta/3)$ should be $\gamma^2 g^2 \delta^2(\Delta - \delta/3)$, as shown correctly a few lines above this. In Eq. [111], the same value is given for all three cases of K_{nm}.

In (*48*), the last part of Eq. [9(c)] is incorrect. The second two parts of Eq. [10(b)] are equal, but they do not equal the first part. In Eq. [11(a)] there should be a coefficient 2 in front of $D_{\perp}$ in the denominator. The formulas for $1 - VR$ in Table 2, and the curve for $1 - VR$ in Fig. 4, are incorrect.

In (*56*), there are mistakes in the derivation of the formula for calculating $TE_{\min}$ from $b_{\max}$. [Also, in Eq. [11], σ_2 should be σ^2, and $(N - N_L/6)$ should be $(N - N_L)/6$.]

In (*57*), the formulas for A_{sd} and A_{fa} are wrong. The formula for A_{gv} in Eq. [6] needs a close parenthesis at the end of the numerator.

In (*40*), in Table 1 the formulas for A_{σ} and *FA* are incorrect, and the letters "rlx" should be removed from the definition of LI_n. (Also, in Eq. [1], the lower limit in the numerator should be $i = 1$, not $i - 1$; and after Eq. [4], $\lambda_{2'''}$ should be $\lambda_{z'''}$.)

In (*58*), the definitions of *FA* (Eq. [4]) and *RA* (Eq. [5]) are incorrect. (Also, in Eq. [1], $b_{high}b_{low}$ should $b_{high} - b_{low}$. In Eq. [2], the left side of the equation should not be in parentheses.)

In (*8*), Eq. [21] was copied incorrectly from the source reference. In the cos term, g_z should be $\sin^{-1}(g_z)$.

In (*1*), the definitions of relative anisotropy (*RA*) (Eq. [9]) and A_{σ} (Eq. [13]) are incorrect.

In (*59*), the definition of A_{sd} (Eq. [5]) is incorrect.

In (*39*), in the appendix, the formula for volume ratio is incorrect.

In (*34*), in the box on page 217, the definition of *FA* is incorrect and the numerators in the definition of *LI* should have bold italic, $\boldsymbol{D}$, to indicate the deviatoric ($\mathbf{D}_{an}$).

Other Mistakes

In (*4*), in Eq. [3] **F** and **G** should be switched. In Eq. [19], either D_{xz} should be -0.00711, or D_{zx} should be 0.00711. In reference 2 the title is incorrect, and the order of the second and third authors is reversed. In reference 4, the page number should be 584, not 1404.

In (*43*), in the paragraph after Eq. [29], $(1 + 2/3\,A)$ should be $(1 + 2A)$.

In (*60*), in Eq. [3b] the *T* should be a superscript to indicate the transpose of the vector.

In (*11*), in the last line of Eq. [7] the term $F_{44} + F_{55} + F_{66}$ should be multiplied by 2.

In (*44*), in Eq. 16, D_x should be D_{xy}.

In (*61*), in Eq. [2] the **D** (bold, tensor) should be D or p (not bold, mean diffusivity).

In (*62*), the 10-direction scheme has 12 directions.

In (*45*), in the Table 1 footnotes, Icos16 should be Icosa6. Reference 6 is in volume 45, not volume 5.

In (*3*), after Eq. 8, $\lambda_?$ should be λ_1, and there should not be a question mark after λ_2.

In (*63*), adding parentheses in Eq. [10], so that $\exp{-b_i\mathbf{r}_i^{T}\mathbf{D}\mathbf{r}_i}$ becomes $\exp(-b_i\mathbf{r}_i^{T}\mathbf{D}\mathbf{r}_i)$, produces a repeat of Eq. [5]. It is not clear if another equation was intended here, or if this equation should have been deleted during a manuscript revision.

In (*54*), the definition of f_r on page 808 should be $(\sqrt{5} - 1)/2$, not $(\sqrt{5 - 1})/2$. In Eq. [6], the argument of $\cos^{-1}$ should be the absolute value of the given expression.

In (*64*), the Fig. 1 legend mentions only a prolate tensor, but the figure includes both oblate and prolate tensors with cylindrical symmetry. Also, below Fig. 1, "rational" should be "relative".

In (*65*), the 12-direction gradient scheme has some typographical errors. It should include all possible combinations of 1, ± 0.5, and 0.

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