Constructing Rotation Matrices using Power Series

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1 Introduction

Although we tend to work with rotation matrices in two or three dimensions, sometimes the question arises about how to generate rotation matrices in arbitrary dimensions. This document describes a method for computing rotation matrices using power series of matrices. The approach is one you see in an undergraduate mathematics course on solving systems of linear differential equations with constant coefficients; for example, see [Bra83, Chapter 3].

1.1 Power Series of Functions

The natural exponential function is introduced in Calculus, namely, $\exp(x) = e^x$, where the base is (approximately) $e \doteq 2.718281828$. The function may be written as a power series

$$\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^k}{k!} + \cdots = \sum_{k=0}^{\infty} \frac{x^k}{k!} \tag{1}$$

The power series is known to converge for any real number x. The formula extends to complex numbers $z = x + iy$, where x and y are real numbers and $i = \sqrt{-1}$,

$$e^z = e^{x+iy} = e^x e^{iy} = \exp(x)\left(\cos(y) + i\sin(y)\right) \tag{2}$$

The term $\exp(x)$ may be written as a power series using Equation (1). The trigonometric terms also have power series representations,

$$\sin(y) = y - \frac{y^3}{3!} + \frac{y^5}{5!} - \cdots = \sum_{k=0}^{\infty} (-1)^k \frac{y^{2k+1}}{(2k+1)!} \tag{3}$$

$$\cos(y) = 1 - \frac{y^2}{2!} + \frac{y^4}{4!} - \cdots = \sum_{k=0}^{\infty} (-1)^k \frac{y^{2k}}{(2k)!} \tag{4}$$

The latter two power series also converge for any real number y.

1.2 Power Series Involving Matrices

The power series representations extend to functions whose inputs are square matrices rather than scalars, taking us into the realm of matrix algebra; for example, see [HJ85]. That is, $\exp(M)$, $\cos(M)$, and $\sin(M)$ are power series of the square matrix M, and they converge for all M.

In particular, we are interested in $\exp(M)$ for square matrix M. A note of caution is in order. The scalar-valued exponential function $\exp(x)$ has various properties that do not immediately extend to the matrix-valued function. For example, we know that

$$\exp(a+b) = e^{a+b} = e^a e^b = e^b e^a = e^{b+a} = \exp(b+a) \tag{5}$$

for any scalars a and b. This formula does not apply to all pairs of matrices A and B. The problem is that matrix multiplication is not commutative, so reversing the order of terms $\exp(A)$ and $\exp(B)$ in the products generally produces different values. It is true, though that

$$\exp(A+B) = \exp(A)\exp(B), \quad \text{when } AB = BA \tag{6}$$

That is, as long as A and B commute in the multiplication, the usual property of power-of-sum-equals-product-of-powers applies.

The power series for $\exp(M)$ of a square matrix M is formally defined as

$$\exp(M) = I + M + \frac{M^2}{2!} + \cdots = \sum_{k=0}^{\infty} \frac{M^k}{k!} \tag{7}$$

and converges for all M. The first term, I, is the identity matrix of the same size as M. The immediate question is how one goes about computing the power series. That is one of the goals of this document and is described next.

1.3 Reduction of the Matrix Power Series

Suppose that the $n \times n$ matrix M is diagonalizable; that is, suppose we may factor $M = PDP^{-1}$, where $D = \text{Diag}(d_1, \ldots, d_n)$ is a diagonal matrix and P is an invertible matrix with inverse P^{-1}. The matrix powers are easily shown to be $M^k = PD^kP^{-1}$, where $D^k = \text{Diag}(d_1^k, \ldots, d_n^k)$. The power series factors as

$$\begin{aligned} \exp(M) &= \textstyle\sum_{k=0}^{\infty} \frac{M^k}{k!} = \sum_{k=0}^{\infty} P\frac{D^k}{k!}P^{-1} \\ &= P\left(\textstyle\sum_{k=0}^{\infty} \frac{D^k}{k!}\right) P^{-1} \\ &= P\,\text{Diag}\left(\textstyle\sum_{k=0}^{\infty} \frac{d_1^k}{k!}, \ldots, \sum_{k=0}^{\infty} \frac{d_n^k}{k!}\right) P^{-1} \\ &= P\,\text{Diag}\left(e^{d_1}, \ldots, e^{d_n}\right) P^{-1} \end{aligned} \tag{8}$$

The expression is valid regardless of whether P and D have real-valued or complex-valued entries. For the purpose of numerical computation, when D has a real-valued entry, d_j, then $\exp(d_j)$ may be computed using any standard mathematics library. Naturally, the computation is only an approximation. When D has a complex-valued entry, $d_j = x_j + iy_j$, then Equation (2) may be used to obtain $\exp(d_j) = \exp(x_j)(\cos(y_j) + i\sin(y_j))$. All of $\exp(x_j)$, $\cos(y_j)$, and $\sin(y_j)$ may be computed using any standard mathematics library.

The problem, though, is that not all matrices M are diagonalizable. A special case that arises often is a real-valued symmetric matrix M. Such matrices have only real-valued eigenvalues and a complete basis of orthonormal eigenvectors. The eigenvalues are the diagonal entries of D and the corresponding eigenvectors become the columns of P. The orthonormality of the eigenvectors guarantees that P is orthogonal, so $P^{-1} = P^{\text{T}}$ (the transpose is the inverse). A more general result is discussed in [HS74, Chapter 6], which applies to all matrices. A brief summary is provided here.

A real-valued matrix S that is diagonalizable is said to be *semisimple*. A real-valued matrix N is *nilpotent* if there exists a power $p \geq 1$ for which $N^p = 0$. Generally, a real-valued matrix M may be uniquely decomposed as $M = S + N$, where S is real-valued and semisimple, N is real-valued and nilpotent, and $SN = NS$. Because S is diagonalizable, we may factor it is $S = PDP^{-1}$, where $D = \text{Diag}(d_1, \ldots, d_n)$ is a diagonal matrix and P is invertible. What this means regarding the exponential function is

$$\exp(M) = \exp(S + N) = \exp(S)\exp(N) = P\,\text{Diag}\left(e^{d_1}, \ldots, e^{d_n}\right) P^{-1} \sum_{k=0}^{p-1} \frac{N^k}{k!} \tag{9}$$

The key here is that the power series for $\exp(N)$ is really a finite sum because N is nilpotent. Equation (9) shows us how to compute $\exp(M)$ for any matrix M; in particular, the equation may be implemented on a computer. Notice that in the special case of a symmetric matrix M, it must be that $M = S$ and $N = 0$.

The discussion here allows for complex numbers. In particular, P and D might have complex-valued entries. Instead, we may factor the $n \times n$ matrix $S = QEQ^{-1}$ as follows. Let S have r real-valued eigenvalues λ_1 through λ_r and c real-valued eigenvalues $\alpha_1 + i\beta_1$ through $\alpha_c + i\beta_c$, where $n = r + c$. We may construct a basis of vectors for $\mathbb{R}^n$ that become the columns of the matrix Q and for which the matrix E has the block-diagonal form

$$E = \begin{bmatrix} \lambda_1 & & & & & & \\ & \ddots & & & & & \\ & & \lambda_r & & & & \\ & & & \begin{bmatrix} \alpha_1 & -\beta_1 \\ \beta_1 & \alpha_1 \end{bmatrix} & & & \\ & & & & \cdots & & \\ & & & & & \begin{bmatrix} \alpha_c & -\beta_c \\ \beta_c & \alpha_c \end{bmatrix} \end{bmatrix} \tag{10}$$

The exponential of E has the block-diagonal form

$$\exp(E) = \begin{bmatrix} e^{\lambda_1} & & & & & & \\ & \ddots & & & & & \\ & & e^{\lambda_r} & & & & \\ & & & e^{\alpha_1} \begin{bmatrix} \cos\beta_1 & -\sin\beta_1 \\ \sin\beta_1 & \cos\beta_1 \end{bmatrix} & & & \\ & & & & \cdots & & \\ & & & & & e^{\alpha_c} \begin{bmatrix} \cos\beta_c & -\sin\beta_c \\ \sin\beta_c & \cos\beta_c \end{bmatrix} \end{bmatrix} \tag{11}$$

The matrix $\exp(M)$ is therefore computed using only real-valued arithmetic. The heart of the construction relies on factoring $M = S + N$, computing the eigenvalues of S, and computing an orthogonal basis for $\mathbb{R}^n$ from S.

1.4 The Cayley-Hamilton Theorem

This is also a useful result that allows a reduction of the power series for $\exp(M)$ to a finite sum. The eigenvalues of an $n \times n$ matrix M are the roots to the *characteristic polynomial*

$$p(t) = \det(M - tI) = p_0 + p_1 t + \cdots + p_n t^n = \sum_{k=0}^{n} p_k t^k \tag{12}$$

where I is the identity matrix. The degree of p is n and the coefficients are p_0 through $p_n = (-1)^n$. The *characteristic equation* is $p(t) = 0$. The *Cayley-Hamilton Theorem* states that if you formally substitute M

into the characteristic equation, you obtain equality,

$$0 = p(M) = p_0 I + p_1 M + \cdots + M^n = \sum_{k=0}^{n} p_k M^k \tag{13}$$

Multiplying this equation by powers of M and reducing everytime the largest power is a multiple of n allows a reduction of the power series for $\exp(M)$ to

$$\exp(M) = \sum_{k=0}^{\infty} \frac{M^k}{k!} = \sum_{k=0}^{n-1} c_k M^k \tag{14}$$

for some coefficients c_0 through c_{n-1}. These coefficients are necessarily functions of the characteristic coefficients p_j for $0 \le j \le n$ but the relationships are at first glance complicated to determine in closed form. This leads us into the topic of *ordinary difference equations*.

1.5 Ordinary Difference Equations

This is a topic whose theory parallels that of ordinary differential equations. It is a large topic that is not discussed in full detail here; a summary of it is provided in [Ebe03, Appendix D]. Generally, one has a sequence of numbers $\{x_k\}_{k=0}^{\infty}$ and a relationship that determines a term in the sequence from the previous n terms:

$$x_{k+n} = f(x_k, \cdots, x_{k+n-1}), \quad k \ge 0 \tag{15}$$

This is an *explicit equation* for x_{k+n}. The equation is said to have degree $n \ge 1$. The *initial conditions* are user-specified x_0 through x_{n-1}. An *implicit equation* is

$$F(x_k, \cdots, x_{k+n-1}, x_{k+n}) = 0, \quad k \ge 0 \tag{16}$$

and are generally more difficult to solve because the x_{k+n} term might occur in such a manner as to prevent solving for it explicitly.

The subtopic of interest here is how to solve ordinary difference equations that are linear and have constant coefficients. The general equation of this form is written with all terms on one side of the equation as if it were implicit, but this is still an explicit equation because we may solve for x_{k+n},

$$p_n x_{k+n} + p_{n-1} x_{k+n-1} + \ldots p_1 x_{k+1} + p_0 x_k = 0 \tag{17}$$

where p_0 through p_n are constants with $p_n \neq 0$. Notice that the coefficients may be used to form the characteristic polynomial described in the previous section, $p(t) = p_0 + p_1 t + \cdots + p_n t^n$ with $p_n = (-1)^n$.

The method of solution for the linear equation with constant coefficients involves computing the roots of the characteristic equation. Let t_1 through t_ℓ be the distinct roots of $p(t) = 0$. Let each root t_j have multiplicity m_j; necessarily, $n = m_1 + \cdots + m_\ell$. The Fundamental Theorem of Algebra states that the polynomial factors into a product,

$$p(t) = \prod_{j=1}^{\ell} (t - t_j)^{m_j} \tag{18}$$

Equation (17) has m_j linearly independent solutions corresponding to t_j, namely,

$$x_k = t_j^k, \quad x_k = k t_j^k, \quad , \cdots, \quad x_k = k^{m_j - 1} t_j^k \tag{19}$$

This is the case even when t_j is a complex-valued root. The general solution to Equation (17) is

$$x_k = \sum_{j=1}^{\ell} \left(\sum_{s=0}^{m_j-1} c_{js} k^s \right) t_j^k, \quad k \geq n \tag{20}$$

where the n coefficients c_{js} are determined from the initial conditions which are the user-specified values x_0 through x_{n-1}.

As it turns out, the finite difference equations and constructions apply equally as well when the x_k are matrices. In this case, the c_{js} of Equation (20) are themselves matrices.

1.6 Generating Rotation Matrices from Skew-Symmetric Matrices

Equation (6) shows how to exponentiate a sum of matrices. As noted, $\exp(A+B) = \exp(A)\exp(B)$ as long as $AB = BA$. In particular, it is the case that $I = \exp(0) = \exp(A + (-A)) = \exp(A)\exp(-A)$, where I is the identity matrix. Thus, we have the formula for inversion of an exponential of a matrix,

$$\exp(A)^{-1} = \exp(-A) \tag{21}$$

The transpose of a sum of matrices is the sum of the transposes of the matrices, a property that also extends to the exponential power series. A consequence is

$$\exp(A)^{\mathrm{T}} = \exp\left(A^{\mathrm{T}}\right) \tag{22}$$

Now consider a skew-symmetric matrix S. Such a matrix has the property $S^{\mathrm{T}} = -S$. Define $R = \exp(S)$. Using Equations (21) and (22),

$$R^{\mathrm{T}} = \exp(S)^{\mathrm{T}} = \exp\left(S^{\mathrm{T}}\right) = \exp(-S) = \exp(S)^{-1} = R^{-1} \tag{23}$$

Because the inverse and transpose of R are the same matrix, R must be an orthogonal matrix. Although in the realm of advanced mathematics, it may be shown that in fact R is a rotation matrix. The essence of the argument is that the space of orthogonal matrices has two connected components, one for which the determinant is 1 (rotation matrices) and one for which the determinant is -1 (reflection matrices). Each component is path connected. The curve of orthogonal matrices $\exp(tS)$ for $t \in [0,1]$ is a path connecting I (the case $t = 0$) and $R = \exp(S)$ (the case $t = 1$), so R and I must have the same determinant, which is 1, and R is therefore a rotation matrix.

2 Rotations Matrices in 2D

The general skew-symmetric matrix in 2D is

$$S = \theta \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -\theta \\ \theta & 0 \end{bmatrix} \tag{24}$$

where θ is any real-valued number. The corresponding rotation matrix is $R = \exp(S)$. The characteristic equation for S is

$$0 = p(t) = \det(S - tI) = t^2 + \theta^2 \tag{25}$$

The Cayley-Hamilton Theorem guarantees that

$$S^2 + \theta^2 I = 0 \tag{26}$$

so that $S^2 = -\theta^2 I$. Higher powers of S are $S^3 = -\theta^2 S$, $S^4 = -\theta^2 S^2 = \theta^4 I$, and so on. Substituting these into the power series for $\exp(S)$ and grouping together the terms involving I and S produces

$$\begin{aligned} R &= \exp(S) \\ &= I + S + \tfrac{S^2}{2!} + \tfrac{S^3}{3!} + \tfrac{S^4}{4!} + \tfrac{S^5}{5!} + \cdots \\ &= I + S - \tfrac{\theta^2}{2!} I - \tfrac{\theta^2}{3!} S + \tfrac{\theta^4}{4!} I + \tfrac{\theta^4}{5!} S - \cdots \\ &= \left(1 - \tfrac{\theta^2}{2!} + \tfrac{\theta^4}{4!} - \cdots\right) I + \left(1 - \tfrac{\theta^2}{3!} + \tfrac{\theta^4}{5!} - \cdots\right) S \\ &= \cos(\theta) I + \left(\tfrac{\sin(\theta)}{\theta}\right) S \\ \\ &= \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \end{aligned} \tag{27}$$

The rotation matrix may be computed using the eigendecomposition method of Equation (8). The eigenvalues of S are $\pm i\theta$, where $i = \sqrt{-1}$. Corresponding eigenvectors are $(\pm i, 1)$. The matrices D, P, and P^{-1} in the decomposition are

$$D = \begin{bmatrix} i\theta & 0 \\ 0 & -i\theta \end{bmatrix}, \quad P = \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix}, \quad P^{-1} = \frac{1}{2i} \begin{bmatrix} 1 & i \\ -1 & i \end{bmatrix} \tag{28}$$

It is easily verified that $S = PDP^{-1}$. The rotation matrix is computed to be

$$\begin{aligned} R &= P \exp(D) P^{-1} \\ \\ &= \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix} \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix} \tfrac{1}{2i} \begin{bmatrix} 1 & i \\ -1 & i \end{bmatrix} \\ \\ &= \begin{bmatrix} \frac{e^{i\theta} + e^{-i\theta}}{2} & -\frac{e^{i\theta} - e^{-i\theta}}{2i} \\ \frac{e^{i\theta} - e^{-i\theta}}{2i} & \frac{e^{i\theta} + e^{-i\theta}}{2} \end{bmatrix} \\ \\ &= \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \end{aligned} \tag{29}$$

where we have used the identities $e^{\pm i\theta} = \cos(\theta) \pm i \sin(\theta)$.

The rotation matrix may also be computed using ordinary finite differences. The linear difference equation is

$$\begin{aligned} &X_{k+2} + \theta^2 X_k = 0, \quad k \geq 0 \\ &X_0 = I, \quad X_1 = S \end{aligned} \tag{30}$$

We know from the construction that $S^k = X_k$. Equation (20) is

$$X_k = (i\theta)^k C_0 + (-i\theta)^k C_1 \tag{31}$$

for unknown coefficient matrices C_0 and C_1. The initial conditions imply

$$\begin{aligned} I &= C_0 + C_1 \\ S &= i\theta C_0 - i\theta C_1 \end{aligned} \tag{32}$$

and have the solution

$$\begin{aligned} C_0 &= \frac{I-(i/\theta)S}{2} \\ C_1 &= \frac{I+(i/\theta)S}{2} \end{aligned} \tag{33}$$

The solution to the linear difference equation is

$$S^k = X_k = (i\theta)^k \frac{I-(i/\theta)S}{2} + (-i\theta)^k \frac{I+(i/\theta)S}{2} \tag{34}$$

When k is even, say, $k = 2p$, Equation (34) reduces to

$$S^{2p} = (-1)^p \theta^{2p} I, \quad p \geq 1 \tag{35}$$

When k is odd, say, $k = 2p+1$, Equation (34) reduces to

$$S^{2p+1} = (-1)^p \theta^{2p} S, \quad p \geq 1 \tag{36}$$

But these powers of S are exactly what we computed manually and substituted into the power series for $\exp(S)$ to produce Equation (27).

3 Rotations Matrices in 3D

The general skew-symmetric matrix in 3D is

$$S = \theta \begin{bmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{bmatrix} \tag{37}$$

where θ, a, b, and c are any real-valued numbers with $a^2 + b^2 + c^2 = 1$. The corresponding rotation matrix is $R = \exp(S)$. The characteristic equation for S is

$$0 = p(t) = \det(S - tI) = -t^3 - \theta^2 t \tag{38}$$

The Cayley-Hamilton Theorem guarantees that

$$-S^3 - \theta^2 S = 0 \tag{39}$$

so that $S^3 = -\theta^2 S$. Higher powers of S are $S^4 = -\theta^2 S^2$, $S^5 = -\theta^2 S^3 = \theta^4 S$, $S^6 = -\theta^2 S^2$, and so on. Substituting these into the power series for $\exp(S)$ and grouping together the terms involving I, S, and S^2 produces

$$\begin{aligned} R &= \exp(S) \\ &= I + S + \tfrac{S^2}{2!} + \tfrac{S^3}{3!} + \tfrac{S^4}{4!} + \tfrac{S^5}{5!} + \tfrac{S^6}{6!} + \cdots \\ &= I + S + \tfrac{1}{2!}S^2 - \tfrac{\theta^2}{3!}S - \tfrac{\theta^2}{4!}S^2 + \tfrac{\theta^4}{5!}S + \tfrac{\theta^4}{6!}S^2 - \cdots \\ &= I + \left(1 - \tfrac{\theta^2}{3!} + \tfrac{\theta^4}{5!} - \cdots\right) S + \left(\tfrac{1}{2!} - \tfrac{\theta^2}{4!} + \tfrac{\theta^4}{6!} - \cdots\right) S^2 \\ &= I + \left(\tfrac{\sin(\theta)}{\theta}\right) S + \left(\tfrac{1-\cos(\theta)}{\theta^2}\right) S^2 \end{aligned} \tag{40}$$

If we define $\hat{S} = S/\theta$, then

$$R = I + \sin(\theta)\hat{S} + (1 - \cos(\theta))\hat{S}^2 \tag{41}$$

which is *Rodrigues' Formula* for a rotation matrix. The angle of rotation is θ and the axis of rotation has unit-length direction $(-c, b, -a)$.

The rotation matrix may also be computed using ordinary finite differences. The linear difference equation is

$$\begin{aligned} &X_{k+3} + \theta^2 X_k = 0, \quad k \geq 0 \\ &X_0 = I, \quad X_1 = S, \quad X_2 = S^2 \end{aligned} \tag{42}$$

We know from the construction that $S^k = X_k$. The roots of the characteristic equation are 1 and $\pm i\theta$. Equation (20) is

$$S^k = X_k = 1^k C_0 + (i\theta)^k C_1 + (-i\theta)^k C_2 \tag{43}$$

for unknown coefficient matrices C_0, C_1, and C_2. The initial conditions imply

$$\begin{aligned} I &= C_0 + C_1 + C_2 \\ S &= C_0 + i\theta C_1 - i\theta C_2 \\ S^2 &= C_0 - \theta^2 C_1 - \theta^2 C_2 \end{aligned} \tag{44}$$

and have the solution

$$\begin{aligned} C_0 &= \tfrac{S^2 + \theta^2 I}{1+\theta^2} \\ C_1 &= \tfrac{(I - C_0) - (i/\theta)(S - C_0)}{2} \\ C_2 &= \tfrac{(I - C_0) + (i/\theta)(S - C_0)}{2} \end{aligned} \tag{45}$$

When k is odd, say, $k = 2p + 1$, Equation (43) reduces to the following using Equation (45)

$$S^{2p+1} = (-1)^p \theta^{2p} S, \quad p \geq 1 \tag{46}$$

When k is even, say, $k = 2p + 2$, Equation (43) reduces to the following using Equation (45)

$$S^{2p+2} = (-1)^p \theta^{2p} S^2, \quad p \geq 1 \tag{47}$$

But these powers of S are exactly what we computed manually and substituted into the power series for $\exp(S)$ to produce Equation (40).

4 Rotations Matrices in 4D

The general skew-symmetric matrix in 4D is

$$S = \theta \begin{bmatrix} 0 & a & b & d \\ -a & 0 & c & e \\ -b & -c & 0 & f \\ -d & -e & -f & 0 \end{bmatrix} \tag{48}$$

where θ, a, b, c, d, e, and f are any real-valued numbers with $a^2+b^2+c^2+d^2+e^2+f^2 = 1$. The corresponding rotation matrix is $R = \exp(S)$. The characteristic equation for S is

$$0 = p(t) = \det(S - tI) = t^4 + \theta^2 t^2 + \theta^4(af - be + cd)^2 = t^4 + \theta^2 t^2 + \theta^4 \delta^2 \tag{49}$$

where $\delta = af - be + cd$. The Cayley-Hamilton Theorem guarantees that

$$S^4 + \theta^2 S^2 + \theta^4 \delta^2 = 0 \tag{50}$$

Computing closed-form expressions for powers of S is simple, much like previous dimensions, when $\delta = 0$. It is more difficult when $\delta \neq 0$. Let us consider the cases separately. In both cases, we assume that $\theta \neq 0$, otherwise $S = 0$ and the rotation matrix is the identity matrix.

4.1 The Case $\delta = 0$

Suppose that $\delta = af - be + cd = 0$; then $S^4 + \theta^2 S^2 = 0$. The closed-form expressions for powers of S are easy to generate. Specifically,

$$\begin{aligned} S^{2p+2} &= (-1)^p \theta^{2p} S^2, \quad p \geq 1 \\ S^{2p+3} &= (-1)^p \theta^{2p} S^3, \quad p \geq 1 \end{aligned} \tag{51}$$

This leads to the power series reduction

$$R = \exp(S) = I + S + \left(\frac{1 - \cos(\theta)}{\theta^2}\right) S^2 + \left(\frac{\theta - \sin(\theta)}{\theta^3}\right) S^3 \tag{52}$$

It is possible for further reduction depending on the entries of S. For example, if $d = e = f = 0$, we effectively have the 3D rotation in (x, y, z) embedded in 4D; the w-component is unchanged by the rotation. The matrix S really satisfies $S^3 + \theta^2 S = 0$, in which case we may replace $S^3 = -\theta^2 S$ in Equation (52) and obtain Equation (40). The fact that S is a "root" of a 3rd-degree polynomial when the characteristic polynomial is 4th-degree is related to the linear algebraic concept of *minimal polynomial*.

Another reduction occurs, for example, when $b = c = d = e = f = 0$. The matrix S satisfies $S^2 + \theta^2 I = 0$ and Equation (52) reduces to Equation (27).

4.2 The Case $\delta \neq 0$

Suppose that $\delta = af - be + cd \neq 0$. The characteristic polynomial $t^4 + \theta^2 t^2 + \theta^4 \delta^2$ is a quadratic polynomial in t^2. We may use the quadratic formula to obtain its roots,

$$t^2 = \frac{-\theta^2 \pm \sqrt{\theta^4 - 4\theta^4\delta^2}}{2} = -\theta^2 \left(\frac{1 \pm \sqrt{1 - 4\delta^2}}{2} \right) \tag{53}$$

Notice that

$$\begin{aligned} 1 - 4\delta^2 &= (a^2 + b^2 + c^2 + d^2 + e^2 + f^2) - 4(af - be + cd)^2 \\ &= \left[(a-f)^2 + (b+e)^2 + (c-d)^2\right]\left[(a+f)^2 + (b-e)^2 + (c+d)^2\right] \\ &= \rho^2 \geq 0 \end{aligned} \tag{54}$$

where

$$\rho = \sqrt{\left[(a-f)^2 + (b+e)^2 + (c-d)^2\right]\left[(a+f)^2 + (b-e)^2 + (c+d)^2\right]} \tag{55}$$

Thus, the right-hand side of Equation (53) is real-valued. Moreover, $1 - 4\delta^2 < 1$, so the right-hand side of Equation (53) consists of two *negative* real numbers. Taking the square roots produces the t-roots for the characteristic equation, all having zero real part,

$$t = \pm i\theta\sqrt{\frac{1-\rho}{2}} =: \pm i\alpha, \quad \pm i\theta\sqrt{\frac{1+\rho}{2}} =: \pm i\beta \tag{56}$$

The values α and β are defined by these equations, both values being positive real numbers with $\alpha \leq \beta$.

4.2.1 The Case $\rho > 0$

Using the linear difference equation approach, the powers of S are

$$S^k = (i\alpha)^k C_0 + (-i\alpha)^k C_1 + (i\beta)^k C_2 + (-i\beta)^k C_3 \tag{57}$$

where the C-matrices are determined by the initial conditions

$$\begin{aligned} I &= C_0 + C_1 + C_2 + C_3 \\ S &= i\alpha C_0 - i\alpha C_1 + i\beta C_2 - i\beta C_3 \\ S^2 &= -\alpha^2 C_0 - \alpha^2 C_1 - \beta^2 C_2 - \beta^2 C_3 \\ S^3 &= -i\alpha^3 C_0 + i\alpha^3 C_1 - i\beta^3 C_2 + i\beta^3 C_3 \end{aligned} \tag{58}$$

The solution is

$$\begin{aligned} C_0 &= \tfrac{\alpha\beta^3 I - i\beta^3 S + \alpha\beta S^2 - i\beta S^3}{2\alpha\beta(\beta^2 - \alpha^2)} \\ C_1 &= \tfrac{\alpha\beta^3 I + i\beta^3 S + \alpha\beta S^2 + i\beta S^3}{2\alpha\beta(\beta^2 - \alpha^2)} \\ C_2 &= \tfrac{-\alpha^3\beta I + i\alpha^3 S - \alpha\beta S^2 + i\alpha S^3}{2\alpha\beta(\beta^2 - \alpha^2)} \\ C_3 &= \tfrac{-\alpha^3\beta I - i\alpha^3 S - \alpha\beta S^2 - i\alpha S^3}{2\alpha\beta(\beta^2 - \alpha^2)} \end{aligned} \tag{59}$$

We may use Equation (57) to compute four consecutive powers of S, namely,

$$\begin{array}{rcl} S^{4p} & = & \frac{\alpha^{4p}(S^2+\beta^2 I)-\beta^{4p}(S^2+\alpha^2 I)}{\beta^2-\alpha^2} \\ S^{4p+1} & = & \frac{\alpha^{4p}(S^3+\beta^2 S)-\beta^{4p}(S^3+\alpha^2 S)}{\beta^2-\alpha^2} \\ S^{4p+2} & = & \frac{-\alpha^{4p+2}(S^2+\beta^2 I)-\beta^{4p+2}(S^2+\alpha^2 I)}{\beta^2-\alpha^2} \\ S^{4p+3} & = & \frac{-\alpha^{4p+2}(S^3+\beta^2 S)-\beta^{4p+2}(S^3+\alpha^2 S)}{\beta^2-\alpha^2} \end{array} \tag{60}$$

for $p \geq 0$. The exponential of S factors to

$$\begin{array}{rcl} \exp(S) & = & \sum_{k=0}^{\infty} \frac{S^k}{k!} \\ & = & \sum_{p=0}^{\infty} \frac{S^{4p}}{(4p)!} + \sum_{p=0}^{\infty} \frac{S^{4p+1}}{(4p+1)!} + \sum_{p=0}^{\infty} \frac{S^{4p+2}}{(4p+2)!} + \sum_{p=0}^{\infty} \frac{S^{4p+3}}{(4p+3)!} \\ & = & \frac{1}{\beta^2-\alpha^2}\left[\left(\sum_{p=0}^{\infty} \frac{\alpha^{4p}}{(4p)!}\right)(S^2+\beta^2 I) - \left(\sum_{p=0}^{\infty} \frac{\beta^{4p}}{(4p)!}\right)(S^2+\alpha^2 I) + \right. \\ & & \left(\sum_{p=0}^{\infty} \frac{\alpha^{4p}}{(4p+1)!}\right)(S^3+\beta^2 S) - \left(\sum_{p=0}^{\infty} \frac{\beta^{4p}}{(4p+1)!}\right)(S^3+\alpha^2 S) - \\ & & \left(\sum_{p=0}^{\infty} \frac{\alpha^{4p+2}}{(4p+2)!}\right)(S^2+\beta^2 I) + \left(\sum_{p=0}^{\infty} \frac{\beta^{4p+2}}{(4p+2)!}\right)(S^2+\alpha^2 I) - \\ & & \left.\left(\sum_{p=0}^{\infty} \frac{\alpha^{4p+2}}{(4p+3)!}\right)(S^3+\beta^2 S) + \left(\sum_{p=0}^{\infty} \frac{\beta^{4p+2}}{(4p+3)!}\right)(S^3+\alpha^2 S)\right] \end{array} \tag{61}$$

This expansion appears to be quite complicated, but the following identities allow us to simplify the expression. Each equation below defines the function $f_j(x)$,

$$\begin{array}{rcccl} f_0(x) & = & \sum_{p=0}^{\infty} \frac{x^{4p}}{(4p)!} & = & \frac{1}{4}\left(e^x+e^{-x}\right)+\frac{1}{2}\cos(x) \\ f_1(x) & = & \sum_{p=0}^{\infty} \frac{x^{4p+1}}{(4p+1)!} & = & \frac{1}{4}\left(e^x-e^{-x}\right)+\frac{1}{2}\sin(x) \\ f_2(x) & = & \sum_{p=0}^{\infty} \frac{x^{4p+2}}{(4p+2)!} & = & \frac{1}{4}\left(e^x+e^{-x}\right)-\frac{1}{2}\cos(x) \\ f_3(x) & = & \sum_{p=0}^{\infty} \frac{x^{4p+3}}{(4p+3)!} & = & \frac{1}{4}\left(e^x-e^{-x}\right)-\frac{1}{2}\sin(x) \end{array} \tag{62}$$

Notice that $f_0(x) = f_1'(x)$, $f_1(x) = f_2'(x)$, $f_2(x) = f_3'(x)$, and $f_3(x) = f_0'(x)$. It is also easy to verify that $\exp(x) = f_0(x) + f_1(x) + f_2(x) + f_3(x)$. Equation (61) becomes

$$\begin{array}{rcl} R = \exp(S) & = & \frac{1}{\beta^2-\alpha^2}\left[f_0(\alpha)(S^2+\beta^2 I) - f_0(\beta)(S^2+\alpha^2 I) + \right. \\ & & \frac{f_1(\alpha)}{\alpha}(S^3+\beta^2 S) - \frac{f_1(\beta)}{\beta}(S^3+\alpha^2 S) - \\ & & f_2(\alpha)(S^2+\beta^2 I) + f_2(\beta)(S^2+\alpha^2 I) - \\ & & \left.\frac{f_3(\alpha)}{\alpha}(S^3+\beta^2 S) + \frac{f_3(\beta)}{\beta}(S^3+\alpha^2 S)\right] \\ & = & \left(\frac{\beta^2\cos(\alpha)-\alpha^2\cos(\beta)}{\beta^2-\alpha^2}\right) I + \left(\frac{\beta^2\sin(\alpha)/\alpha-\alpha^2\sin(\beta)/\beta}{\beta^2-\alpha^2}\right) S + \\ & & \left(\frac{\cos(\alpha)-\cos(\beta)}{\beta^2-\alpha^2}\right) S^2 + \left(\frac{\sin(\alpha)/\alpha-\sin(\beta)/\beta}{\beta^2-\alpha^2}\right) S^3 \end{array} \tag{63}$$

4.2.2 The Case $\rho = 0$

Let $\rho = 0$. Based on Equation (54), the only time this can happen is when $(a, b, c) = \pm(f, -e, d)$. This condition implies $a^2 + b^2 + c^2 = 1/2$ and $\delta^2 = 1/4$. The t-roots are $\pm i\theta/\sqrt{2}$, each one having multiplicity 2.

Define $\alpha = \theta/\sqrt{2}$. Using the linear difference equation approach, the powers of S are

$$S^k = (i\alpha)^k C_0 + (-i\alpha)^k C_1 + k(i\alpha)^k C_2 + k(-i\alpha)^k C_3 \tag{64}$$

where the C-matrices are determined by the initial conditions

$$\begin{aligned} I &= C_0 + C_1 \\ S &= i\alpha(C_0 - C_1 + C_2 - C_3) \\ S^2 &= -\alpha^2(C_0 + C_1 + 2C_2 + 2C_3) \\ S^3 &= -i\alpha^3(C_0 - C_1 + 3C_2 - 3C_3) \end{aligned} \tag{65}$$

The solution is

$$\begin{aligned} C_0 &= \tfrac{I}{2} - \tfrac{3iS}{2\sqrt{2}\,\theta} - \tfrac{iS^3}{\sqrt{2}\,\theta^3} \\ C_1 &= \tfrac{I}{2} + \tfrac{3iS}{2\sqrt{2}\,\theta} + \tfrac{iS^3}{\sqrt{2}\,\theta^3} \\ C_2 &= -\tfrac{I}{4} + \tfrac{iS}{2\sqrt{2}\,\theta} - \tfrac{S^2}{2\theta^2} + \tfrac{iS^3}{\sqrt{2}\,\theta^3} \\ C_3 &= -\tfrac{I}{4} - \tfrac{iS}{2\sqrt{2}\,\theta} - \tfrac{S^2}{2\theta^2} - \tfrac{iS^3}{\sqrt{2}\,\theta^3} \end{aligned} \tag{66}$$

We may use Equation (64) to compute four consecutive powers of S, namely,

$$\begin{aligned} S^{4p} &= \alpha^{4p} I - 4p\alpha^{4p}\left(\tfrac{I}{2} + \tfrac{S^2}{2\alpha^2}\right) \\ S^{4p+1} &= \alpha^{4p+1}\tfrac{S}{\alpha} - 4p\alpha^{4p+1}\left(\tfrac{S}{2\alpha} + \tfrac{S^3}{2\alpha^3}\right) \\ S^{4p+2} &= \alpha^{4p+2}\tfrac{S^2}{\alpha^2} + 4p\alpha^{4p+2}\left(\tfrac{I}{2} + \tfrac{S^2}{2\alpha^2}\right) \\ S^{4p+3} &= \alpha^{4p+3}\tfrac{S^3}{\alpha^3} + 4p\alpha^{4p+3}\left(\tfrac{S}{2\alpha} + \tfrac{S^3}{2\alpha^3}\right) \end{aligned} \tag{67}$$

for $p \geq 0$. Define $\hat{S} = S/\alpha$. The exponential of S factors to

$$\begin{aligned} \exp(S) &= \textstyle\sum_{k=0}^{\infty} \frac{S^k}{k!} \\ &= \textstyle\sum_{p=0}^{\infty} \frac{S^{4p}}{(4p)!} + \sum_{p=0}^{\infty} \frac{S^{4p+1}}{(4p+1)!} + \sum_{p=0}^{\infty} \frac{S^{4p+2}}{(4p+2)!} + \sum_{p=0}^{\infty} \frac{S^{4p+3}}{(4p+3)!} \\ &= \left(\textstyle\sum_{p=0}^{\infty} \frac{\alpha^{4p}}{(4p)!}\right) I - \left(\sum_{p=0}^{\infty} \frac{4p\alpha^{4p}}{(4p)!}\right)\left(\frac{I}{2} + \frac{\hat{S}^2}{2}\right) + \\ &\quad \left(\textstyle\sum_{p=0}^{\infty} \frac{\alpha^{4p+1}}{(4p+1)!}\right) \hat{S} - \left(\sum_{p=0}^{\infty} \frac{4p\alpha^{4p+1}}{(4p+1)!}\right)\left(\frac{\hat{S}}{2} + \frac{\hat{S}^3}{2}\right) + \\ &\quad \left(\textstyle\sum_{p=0}^{\infty} \frac{\alpha^{4p+2}}{(4p+2)!}\right) \hat{S}^2 + \left(\sum_{p=0}^{\infty} \frac{4p\alpha^{4p+2}}{(4p+2)!}\right)\left(\frac{I}{2} + \frac{\hat{S}^2}{2}\right) + \\ &\quad \left(\textstyle\sum_{p=0}^{\infty} \frac{\alpha^{4p+3}}{(4p+3)!}\right) \hat{S}^3 + \left(\sum_{p=0}^{\infty} \frac{4p\alpha^{4p+3}}{(4p+3)!}\right)\left(\frac{\hat{S}}{2} + \frac{\hat{S}^3}{2}\right) \end{aligned} \tag{68}$$

We may simplify this using the definitions for $f_j(x)$ and the following identities,

$$\begin{aligned} g_0(x) &= \textstyle\sum_{p=0}^{\infty} \frac{4px^{4p}}{(4p)!} &&= xf_3(x) \\ g_1(x) &= \textstyle\sum_{p=0}^{\infty} \frac{4px^{4p+1}}{(4p+1)!} &&= xf_0(x) - f_1(x) \\ g_2(x) &= \textstyle\sum_{p=0}^{\infty} \frac{4px^{4p+2}}{(4p+2)!} &&= xf_1(x) - 2f_2(x) \\ g_3(x) &= \textstyle\sum_{p=0}^{\infty} \frac{4px^{4p+3}}{(4p+3)!} &&= xf_2(x) - 3f_3(x) \end{aligned} \tag{69}$$

Notice that $g_0(x) = g_1'(x)$, $g_1(x) = g_2'(x)$, and $g_2(x) = g_3'(x)$. Equation (68) becomes

$$\begin{aligned} R = \exp(S) &= \left(f_0(\alpha) - \tfrac{g_0(\alpha)}{2} + \tfrac{g_2(\alpha)}{2}\right) I + \left(f_1(\alpha) - \tfrac{g_1(\alpha)}{2} + \tfrac{g_3(\alpha)}{2}\right) \hat{S} + \\ &\quad \left(f_2(\alpha) - \tfrac{g_0(\alpha)}{2} + \tfrac{g_2(\alpha)}{2}\right) \hat{S}^2 + \left(f_3(\alpha) - \tfrac{g_1(\alpha)}{2} + \tfrac{g_3(\alpha)}{2}\right) \hat{S}^3 \\ &= \left(\tfrac{2\cos(\alpha)+\alpha\sin(\alpha)}{2}\right) I + \left(\tfrac{3\sin(\alpha)-\alpha\cos(\alpha)}{2\alpha}\right) S + \\ &\quad \left(\tfrac{\sin(\alpha)}{2\alpha}\right) S^2 + \left(\tfrac{\sin(\alpha)-\alpha\cos(\alpha)}{2\alpha^3}\right) S^3 \end{aligned} \tag{70}$$

4.3 Summary of the Formulas

We start with the skew-symmetric matrix

$$S = \theta \begin{bmatrix} 0 & a & b & d \\ -a & 0 & c & e \\ -b & -c & 0 & f \\ -d & -e & -f & 0 \end{bmatrix} \tag{71}$$

where $a^2 + b^2 + c^2 + d^2 + e^2 + f^2 = 1$. Define

$$\delta = af - be + cd, \quad \rho = \sqrt{1 - 4\delta^2}, \quad \alpha = \theta\sqrt{\frac{1-\rho}{2}}, \quad \beta = \theta\sqrt{\frac{1+\rho}{2}} \tag{72}$$

Equation (63) really is the most general formula for the rotation matrix R corresponding to a skew-symmetric matrix S. To repeat that formula,

$$\begin{aligned} R &= \left(\tfrac{\beta^2\cos(\alpha)-\alpha^2\cos(\beta)}{\beta^2-\alpha^2}\right) I + \left(\tfrac{\beta^2\sin(\alpha)/\alpha-\alpha^2\sin(\beta)/\beta}{\beta^2-\alpha^2}\right) S \\ &\quad + \left(\tfrac{\cos(\alpha)-\cos(\beta)}{\beta^2-\alpha^2}\right) S^2 + \left(\tfrac{\sin(\alpha)/\alpha-\sin(\beta)/\beta}{\beta^2-\alpha^2}\right) S^3 \end{aligned} \tag{73}$$

This equation was constructed for when $\beta > \alpha > 0$. However, when $\alpha = 0$, Equation(73) reduces to Equation (52), with only the name change from θ to β,

$$R = I + S + \left(\tfrac{1-\cos(\beta)}{\beta^2}\right) S^2 + \left(\tfrac{\beta-\sin(\beta)}{\beta^3}\right) S^3 \tag{74}$$

The evaluation of $\sin(\alpha)/\alpha$ at $\alpha = 0$ is done in the limiting sense, $\lim_{\alpha\to 0} \sin(\alpha)/\alpha = 1$. Equation (70) was for the case $\beta = \alpha$ but may be obtained also from Equation (73) in the limiting sense as $\beta \to \alpha$. l'Hôpital's Rule may be applied to the coefficients of I, S, S^2, and S^3 to obtain the coefficients in Equation (70),

$$\begin{aligned} R &= \left(\tfrac{2\cos(\alpha)+\alpha\sin(\alpha)}{2}\right) I + \left(\tfrac{3\sin(\alpha)-\alpha\cos(\alpha)}{2\alpha}\right) S \\ &\quad + \left(\tfrac{\sin(\alpha)}{2\alpha}\right) S^2 + \left(\tfrac{\sin(\alpha)-\alpha\cos(\alpha)}{2\alpha^3}\right) S^3 \end{aligned} \tag{75}$$

4.4 Source Code for Random Generation

Here is some sample code to illustrate Equation (73) when $\beta \neq \alpha$.

```
void RandomRotation4D_BetaNotEqualAlpha ()
{
    double a = Mathd::SymmetricRandom();  // number is in [-1,1)
    double b = Mathd::SymmetricRandom();  // number is in [-1,1)
    double c = Mathd::SymmetricRandom();  // number is in [-1,1)
    double d = Mathd::SymmetricRandom();  // number is in [-1,1)
    double e = Mathd::SymmetricRandom();  // number is in [-1,1)
    double f = Mathd::SymmetricRandom();  // number is in [-1,1)
    Matrix4d S
    (
        0.0, a,   b,   d,
        -a,  0.0, c,   e,
        -b,  -c,  0.0, f,
        -d,  -e,  -f,  0.0
     );

    double theta = Mathd::Sqrt(a*a + b*b + c*c + d*d + e*e + f*f);
    double invLength = 1.0/theta;
    a *= invLength;
    b *= invLength;
    c *= invLength;
    d *= invLength;
    e *= invLength;
    f *= invLength;

    double delta = a*f - b*e + c*d;
    double delta2 = delta*delta;
    double p = Mathd::Sqrt(1.0 - 4.0*delta2);
    double alpha = theta*Mathd::Sqrt(0.5*(1.0 - p));
    double beta = theta*Mathd::Sqrt(0.5*(1.0 + p));
    double invDenom = 1.0/(beta*beta - alpha*alpha);
    double cosa = Mathd::Cos(alpha);
    double sina = Mathd::Sin(alpha);
    double cosb = Mathd::Cos(beta);
    double sinb = Mathd::Sin(beta);

    double k0 = (beta*beta*cosa - alpha*alpha*cosb)*invDenom;
    double k1 = (beta*beta*sina/alpha - alpha*alpha*sinb/beta)*invDenom;
    double k2 = (cosa - cosb)*invDenom;
    double k3 = (sina/alpha - sinb/beta)*invDenom;

    Matrix4d I = Matrix4d::IDENTITY;
    Matrix4d S2 = S*S;
    Matrix4d S3 = S*S2;
```

```
    Matrix4d R = k0*I + k1*S + k2*S2 + k3*S3;  // The random rotation matrix.

    // Sanity checks.
    Matrix4d S4 = S*S3;
    double theta2 = theta*theta;
    double theta4 = theta2*theta2;
    Matrix4d zero0 = S4 + theta2*S2 + (theta4*delta2)*I;  // = the zero matrix
    double one = R.Determinant();  // = 1
    Matrix4d zero1 = R.TransposeTimes(R) - I;  // = the zero matrix
}
```

Here is some sample code to illustrate the case when $\beta = \alpha$.

```
void RandomRotation4D_BetaEqualAlpha ()
{
    double a = Mathd::SymmetricRandom();  // number is in [-1,1)
    double b = Mathd::SymmetricRandom();  // number is in [-1,1)
    double c = Mathd::SymmetricRandom();  // number is in [-1,1)
    double mult = Mathd::Sqrt(0.5)/Mathd::Sqrt(a*a + b*b + c*c);
    a *= mult;
    b *= mult;
    c *= mult;
    double d = c;
    double e = -b;
    double f = a;
    double theta = Mathd::SymmetricRandom();
    Matrix4d S
    (
        0.0, a,   b,   d,
        -a,  0.0, c,   e,
        -b,  -c,  0.0, f,
        -d,  -e,  -f,  0.0
     );
    S *= theta;

    double lensqr = a*a + b*b + c*c + d*d + e*e + f*f;  // = 1
    double delta = a*f - b*e + c*d;  // = 1/2
    double delta2 = delta*delta;  // = 1/4
    double discr = 1.0 - 4.0*delta2;  // = 0
    double p = Mathd::Sqrt(Mathd::FAbs(discr)); // = 0
    double alpha = theta*Mathd::Sqrt(0.5);
    double cosa = Mathd::Cos(alpha);
    double sina = Mathd::Sin(alpha);

    double k0 = (2.0*cosa + alpha*sina)/2.0;
    double k1 = (3.0*sina - alpha*cosa)/(2.0*alpha);
    double k2 = sina/(2.0*alpha);
    double k3 = (sina - alpha*cosa)/(2.0*alpha*alpha*alpha);
```

```
    Matrix4d I = Matrix4d::IDENTITY;
    Matrix4d S2 = S*S;
    Matrix4d S3 = S*S2;
    Matrix4d R = k0*I + k1*S + k2*S2 + k3*S3;  // The random rotation matrix.

    // Sanity checks.
    Matrix4d S4 = S*S3;
    double theta2 = theta*theta;
    double theta4 = theta2*theta2;
    Matrix4d zero0 = S4 + theta2*S2 + (theta4*delta2)*I;  // = the zero matrix
    double one = R.Determinant();  // = 1
    Matrix4d zero1 = R.TransposeTimes(R);  // = the zero matrix
}
```

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