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EXPRESSION FOR A GENERAL ELEMENT OF AN SO(n) MATRIX

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We derive the expression for a general element of an SO(n) matrix. All elements are obtained from a single element of the matrix. This has applications in recently developed methods for computing Lyapunov exponents.

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1. Introduction. Matrix representations of the SO(n) group have played an important role in mathematical physics [5, 6]. They continue to be used in many fields to this day [4, 7, 8]. They also play a crucial role in new methods for computing Lyapunov exponents [2, 3].

In this paper, we obtain the expression for a general element of an SO(n) matrix $Q^{(n)}$ for $n \geq 3$. This offers significant advantages in generalizing the recent Lyapunov spectrum calculation methods [2, 3] to higher dimensions. We demonstrate that expressions for all elements can be obtained from the expression of a single matrix element by suitable operations. As an example of the application of these results, we derive the elements of an SO(3) matrix in Section 3. The standard expressions are obtained as expected.

2. General element of an SO(n) matrix. In this section, we derive the expression for a general element of an SO(n) matrix denoted by $Q^{(n)}$ (for $n \geq 3$). In all the expressions below, it is implicitly assumed that $n \geq 3$.

We start by deriving the expression for the element $Q_{1n}^{(n)}$. Then we prove that all other elements of $Q^{(n)}$ can be obtained from this single element and give explicit expressions for these elements. This method is based on the representation of the group SO(n) as a product of $n(n-1)/2$ $n \times n$ matrices, which are simple rotations in the $(i-j)$th coordinates [1].

Proposition 2.1. *An SO(n) matrix $Q^{(n)}$ can be represented as the following product of simple rotations (see [1]):*

$$Q^{(n)} = O^{(1,2)} O^{(1,3)} \cdots O^{(1,n)} \cdots O^{(n-1,n)}, \tag{2.1}$$

where $O^{(i,j)}$ is given as

$$O_{kl}^{(i,j)} = \begin{cases} 1, & \textit{if } k = 1 \neq i, j; \\ \cos\theta_r, & \textit{if } k = l = i \textit{ or } j; \\ \sin\theta_r, & \textit{if } k = i,\ l = j; \\ -\sin\theta_r, & \textit{if } k = j,\ l = i; \\ 0, & \textit{otherwise}, \end{cases} \tag{2.2}$$

where $r = (i-1)(2n-i)/2 + j - i$.

Let

$$\begin{aligned} T^{(1)} &= O^{(1,2)}O^{(1,3)}\cdots O^{(1,n)}, \\ T^{(2)} &= O^{(2,3)}O^{(2,4)}\cdots O^{(2,n)}, \\ &\vdots \\ T^{(k)} &= O^{(k,k+1)}O^{(k,k+2)}\cdots O^{(k,n)}, \\ &\vdots \\ T^{(n-1)} &= O^{(n-1,n)}. \end{aligned} \tag{2.3}$$

We see that the matrix $T^{(1)}$ depends only on the first $(n-1)$ θ_i's, namely, θ_1, $\theta_2, \ldots, \theta_{n-1}$, and the matrix $T^{(2)}$ depends only on the next $(n-2)$ θ_i's, namely, $\theta_n, \theta_{n+1}, \ldots, \theta_{2n-3}$, and so on. Finally, the matrix $T^{(n-1)}$ depends only on one θ_i, namely, $\theta_{n(n-1)/2}$. Thus, a general matrix $T^{(k)}$ is parameterized by the following θ_i's, namely, $\theta_{m(n,k)}, \theta_{m(n,k)+1}, \ldots, \theta_{p(n,k)}$, where $m(n,k)$ and $p(n,k)$ are given by

$$m(n,k) = \frac{(k-1)(2n-k)+2}{2}, \tag{2.4}$$

$$p(n,k) = \frac{k(2n-k-1)}{2}. \tag{2.5}$$

Therefore,

$$Q^{(n)} = T^{(1)}T^{(2)}\cdots T^{(n-1)}. \tag{2.6}$$

The matrix $T^{(k)}$ $(k = 1, 2, \ldots, n-1)$ is given by

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & & R^{(k)} & \\ 0 & & & \end{bmatrix}, \tag{2.7}$$

where $R^{(k)}$ is an $(n-k+1)\times(n-k+1)$ matrix parameterized by $\theta_{m(n,k)+1}$, $\theta_{m(n,k)+2}, \ldots, \theta_{p(n,k)}$, where $m(n,k)$ and $p(n,k)$ are given by (2.4) and (2.5), respectively. The elements of $R^{(k)}$ are given as follows:

$$R_{11}^{(k)} = \prod_{r=m(n,k)}^{p(n,k)} \cos\theta_r, \tag{2.8}$$

$$R_{12}^{(k)} = \sin\theta_{m(n,k)}, \tag{2.9}$$

and for $j = 3,4,\dots,n-(k-1)$,

$$R_{1j}^{(k)} = \left(\prod_{r=0}^{j-3} \cos\theta_{m(n,k)+r}\right) \sin\theta_{m(n,k)+j-2}. \tag{2.10}$$

The second row ($j = 1,2,\dots,n-(k-1)$) is given by

$$R_{2j}^{(k)} = \frac{\partial}{\partial\theta_{m(n,k)}} R_{1j}^{(k)}. \tag{2.11}$$

The rest of the rows ($i = 3,4,\dots,n-(k-1)$ and $j = 1,2,\dots,n-(k-1)$) are given by

$$R_{ij}^{(k)} = \frac{\partial}{\partial\theta_{m(n,k)+i-2}} \mathcal{I}_{ij}^{(k)}, \tag{2.12}$$

where $\mathcal{I}_{ij}^{(k)}$ = Coefficient of $\prod_{r=0}^{i-3}\cos\theta_{m(n,k)+r}$ in $R_{1j}^{(k)}$.

Putting everything together, from (2.6) we have the following lemma.

Lemma 2.2. *Let $Q^{(n)}$ be an* SO(n) *matrix ($n \geq 3$). Then the element $Q_{1n}^{(n)}$ is given by the expression*

$$Q_{1n}^{(n)} = \sum_{j_{n-2}=2}^{3} \sum_{j_{n-3}=2}^{4} \cdots \sum_{j_2=2}^{n-1} \sum_{j_1=2}^{n} R_{1,j_1}^{(1)} R_{j_1-1,j_2}^{(2)} R_{j_2-1,j_3}^{(3)} \cdots R_{j_{n-2}-1,2}, \tag{2.13}$$

where $j_{n-1} = 2$.

Next, we prove that all other elements of $Q^{(n)}$ can be obtained from the single element $Q_{1n}^{(n)}$ (derived above). To show this, we need some preliminary results contained in Lemmas 2.3 and 2.4 proved below.

Lemma 2.3. *Consider a general* SO(n) *matrix $Q^{(n)}$ ($n \geq 3$). The expressions for $Q_{in}^{(n)}$'s, $i = 1,2,\dots,n-1$, do not involve the term* $\cos\theta_{p(n,1)}$ $(= \cos\theta_{n-1})$ *in them.*

Proof. We can write the matrix $Q^{(n)}$ as

$$Q^{(n)} = R^{(1)}\Gamma \quad (\text{since } T^{(1)} = R^{(1)}), \tag{2.14}$$

where Γ is of the form

$$\Gamma = T^{(2)}T^{(3)}\cdots T^{(n-1)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & A^{(n-1)} & \\ 0 & & & \end{bmatrix}. \tag{2.15}$$

Here $A^{(n-1)}$ is a general $\mathrm{SO}(n-1)$ matrix parameterized by $\theta_n, \theta_{n+1}, \ldots, \theta_{n(n-1)/2}$. Thus, $Q_{in}^{(n)}$ $(i = 1,2,\ldots,n-1)$ is given by

$$Q_{in}^{(n)} = \sum_{k=2}^{n} R_{ik}^{(1)} A_{k-1,n-1}^{(n-1)}. \tag{2.16}$$

From this equation, we see that $R_{i1}^{(1)}$'s $(i = 1,2,\ldots,n-1)$ are absent in the expressions for $Q_{in}^{(n)}$ $(i = 1,2,\ldots,n-1)$. Also, by (2.9), (2.10), (2.11), and (2.12), which give the expressions for $R_{ij}^{(k)}$'s, we see that the term $\cos\theta_{n-1}$ is absent in all the $R_{ik}^{(1)}$'s, where $i = 1,2,\ldots,n-1$ and $k = 2,3,\ldots,n$. Finally, $A^{(n-1)}$ is parameterized by $\theta_n, \theta_{n+1}, \ldots, \theta_{n(n-1)/2}$ and hence does not contain the term $\cos\theta_{n-1}$. Therefore, $Q_{in}^{(n)}$ $(i = 1,2,\ldots,n-1)$ does not involve the term $\cos\theta_{n-1}$. This proves the lemma. □

Lemma 2.4. *For $n \geq 3$, $Q_{nn}^{(n)} = \prod_{k=1}^{n-1}\cos\theta_{p(n,k)}$, where*

$$p(n,k) = \frac{k(2n-k-1)}{2}. \tag{2.17}$$

This lemma is easily proved by mathematical induction and hence we omit the proof.

We are now in a position to prove that we can obtain all rows of $Q^{(n)}$ given only the first row.

Lemma 2.5. *Let $Q^{(n)}$ be an $\mathrm{SO}(n)$ matrix $(n \geq 3)$. Let $Q_{1i}^{(n)}$, $i = 1,2,\ldots,n$, be its first row. Then the second row is given by the following equation:*

$$Q_{2l}^{(n)} = \frac{\partial Q_{1l}^{(n)}}{\partial\theta_1}, \quad l = 1,2,\ldots,n. \tag{2.18}$$

The other rows are given by the following expression:

$$Q_{il}^{(n)} = \frac{\partial \mathcal{B}_{il}^{(n)}}{\partial\theta_{i-1}}, \quad i = 3,4,\ldots,n;\ l = 1,2,\ldots,n, \tag{2.19}$$

where

$$\mathcal{B}_{il}^{(n)} = \textit{Coefficient of } \prod_{r=1}^{i-2}\cos\theta_r \textit{ in } Q_{1l}^{(n)}. \tag{2.20}$$

Proof. A general SO(n) matrix $Q^{(n)}$ is given by

$$Q^{(n)} = T^{(1)}\Gamma, \tag{2.21}$$

where $T^{(1)}$ and Γ are given by (2.3) and (2.15), respectively. The matrix $T^{(1)}$ is parameterized by the following $(n-1)$ θ's, namely, $\theta_1, \theta_2, \ldots, \theta_{n-1}$ while Γ is given by (2.15), where $A^{(n-1)}$ is an SO($n-1$) matrix, parameterized by $(n-1)(n-2)/2$ θ's, namely, $\theta_n, \theta_{n+1}, \ldots, \theta_{n(n-1)/2}$. Thus, $Q^{(n)}_{i1}$, $i = 1, 2, \ldots, n$, is given by

$$Q^{(n)}_{i1} = R^{(1)}_{i1}. \tag{2.22}$$

Using this equation and (2.11), we obtain

$$Q^{(n)}_{21} = \frac{\partial Q^{(n)}_{11}}{\partial \theta_1}. \tag{2.23}$$

Also, from (2.12), we have

$$R^{(1)}_{i1} = \frac{\partial \mathcal{I}^{(1)}_{i1}}{\partial \theta_{i-1}}, \quad i = 3, 4, \ldots, n, \tag{2.24}$$

where (see (2.22) and (2.20))

$$\mathcal{I}^{(1)}_{i1} = \mathcal{B}^{(n)}_{i1}. \tag{2.25}$$

Thus,

$$\frac{\partial \mathcal{B}^{(1)}_{i1}}{\partial \theta_{i-1}} = \frac{\partial \mathcal{I}^{(1)}_{i1}}{\partial \theta_{i-1}} = R^{(1)}_{i1} = Q^{(n)}_{i1}, \quad i = 3, 4, \ldots, n. \tag{2.26}$$

Now, for $l = 2, 3, \ldots, n$, we have

$$Q^{(n)}_{il} = \sum_{k=2}^{n} R^{(1)}_{ik} A^{(n-1)}_{k-1,l-1}. \tag{2.27}$$

Putting $i = 1$, we get

$$Q^{(n)}_{1l} = \sum_{k=2}^{n} R^{(1)}_{1k} A^{(n-1)}_{k-1,l-1}. \tag{2.28}$$

Since $A^{(n-1)}_{k-1,l-1}$'s do not involve the first $(n-1)$ θ's, namely, $\theta_1, \theta_2, \ldots, \theta_{n-1}$, we obtain (for $k = 2, 3, \ldots, n$)

$$\frac{\partial}{\partial \theta_1}\left(R^{(1)}_{1k} A^{(n-1)}_{k-1,l-1}\right) = R^{(1)}_{2k} A^{(n-1)}_{k-1,l-1}. \tag{2.29}$$

Summing over k ($k = 2, 3, \ldots, n$) and using (2.28) and (2.23), we get

$$\frac{\partial}{\partial \theta_1} Q^{(n)}_{1l} = Q^{(n)}_{2l}, \quad l = 1, 2, \ldots, n. \tag{2.30}$$

Thus, the second row of $Q^{(n)}$, namely, $Q_{2l}^{(n)}$ $(l = 1,2,\dots,n)$ obeys the hypothesis (2.18). We will now prove the hypothesis for the rest of its rows.

Let

$$\mathcal{I}_{il}^{(1)} = \text{Coefficient of } \prod_{r=1}^{i-2} \cos\theta_r \text{ in } R_{1l}^{(1)}, \quad i = 3,4,\dots,n, \tag{2.31}$$

$$\mathcal{C}_{ik} = \text{Coefficient of } \prod_{r=1}^{i-2} \cos\theta_r \text{ in } R_{1k}^{(1)} A_{k-1,l-1}^{(n-1)}, \quad i = 3,4,\dots,n;\ k = 2,3,\dots,n. \tag{2.32}$$

Therefore, (see (2.28) and (2.20))

$$\sum_{k=2}^{n} \mathcal{C}_{ik} = \mathcal{B}_{il}^{(n)}. \tag{2.33}$$

Since $A_{k-1,l-1}^{(n-1)}$'s do not involve $\theta_1, \theta_2, \dots, \theta_{n-1}$, we have from (2.32)

$$\mathcal{C}_{ik} = A_{k-1,l-1}^{(n-1)} \mathcal{I}_{ik}^{(1)}, \tag{2.34}$$

where $\mathcal{I}_{ik}^{(1)} = \text{Coefficient of } \prod_{r=1}^{i-2} \cos\theta_r \text{ in } R_{1k}^{(1)}$.

Thus, (see (2.12))

$$\frac{\partial \mathcal{C}_{ik}}{\partial \theta_{i-1}} = A_{k-1,l-1}^{(n-1)} \frac{\partial \mathcal{I}_{ik}^{(1)}}{\partial \theta_{i-1}} = A_{k-1,l-1}^{(n-1)} R_{ik}^{(1)}. \tag{2.35}$$

Summing both sides over k $(k = 2,3,\dots,n)$, we obtain

$$\sum_{k=2}^{n} \frac{\partial \mathcal{C}_{ik}}{\partial \theta_{i-1}} = \sum_{k=2}^{n} R_{ik}^{(1)} A_{k-1,l-1}^{(n-1)} = Q_{il}^{(n)}. \tag{2.36}$$

But, from (2.33),

$$\sum_{k=2}^{n} \frac{\partial \mathcal{C}_{ik}}{\partial \theta_{i-1}} = \frac{\partial \left(\sum_{k=2}^{n} \mathcal{C}_{ik} \right)}{\partial \theta_{i-1}} = \frac{\partial \mathcal{B}_{il}^{(n)}}{\partial \theta_{i-1}}. \tag{2.37}$$

Thus,

$$\frac{\partial \mathcal{B}_{il}^{(n)}}{\partial \theta_{i-1}} = Q_{il}^{(n)}, \tag{2.38}$$

where $\mathcal{B}_{il}^{(n)} = \text{Coefficient of } \prod_{r=1}^{i-2} \cos\theta_r \text{ in } Q_{1l}^{(n)}$ for $l = 2,3,\dots,n$.

Combining the above equation with (2.26), we obtain the following:

$$Q_{il}^{(n)} = \frac{\partial \mathcal{B}_{il}^{(n)}}{\partial \theta_{i-1}}, \quad i = 3,4,\dots,n;\ l = 1,2,\dots,n, \tag{2.39}$$

where $\mathcal{B}_{il}^{(n)} = \text{Coefficient of } \prod_{r=1}^{i-2} \cos\theta_r \text{ in } Q_{1l}^{(n)}$. Thus, (2.30) and (2.39) prove the lemma. □

We next prove a result analogous to Lemma 2.5, but for columns instead of rows. Combining Lemmas 2.5 and 2.6 will give us the desired result of obtaining all elements of $Q^{(n)}$ from a single element.

Lemma 2.6. *For $n \geq 3$, given the nth column of $Q^{(n)}$, the $(n-1)$th column is given by the following expression:*

$$Q^{(n)}_{i,n-1} = \frac{\partial Q^{(n)}_{in}}{\partial \theta_{p(n,n-1)}}, \quad i = 1,2,\ldots,n. \tag{2.40}$$

The other columns are given by

$$Q^{(n)}_{il} = \frac{\partial \mathcal{D}^{(n)}_{il}}{\partial \theta_{p(n,l)}}, \quad i = 1,2,\ldots,n;\ l = 1,2,\ldots,n-2, \tag{2.41}$$

where $\mathcal{D}^{(n)}_{il}$ = Coefficient of $\prod_{m=l+1}^{n-1} \cos\theta_{p(n,m)}$ in $Q^{(n)}_{in}$.

The proof of this lemma is by induction and is straightforward (though laborious). So we omit the proof.

Lemma 2.6 implies that given the last column of $Q^{(n)}$, we can derive the other columns. In particular, given $Q^{(n)}_{1n}$ (Lemma 2.2), we can obtain the first row. Once the first row is known, using Lemma 2.5, all other rows can be derived. Therefore, we see that from one element of $Q^{(n)}$, namely, $Q^{(n)}_{1n}$ we can generate the whole SO(n) matrix by performing suitable operations. Thus we have proved the following theorem.

Theorem 2.7. *Consider an $n \times n$ SO(n) matrix $Q^{(n)}$ ($n \geq 3$). The expression for $Q^{(n)}_{1n}$ is given by*

$$Q^{(n)}_{1n} = \sum_{j_{n-2}=2}^{3} \sum_{j_{n-3}=2}^{4} \cdots \sum_{j_2=2}^{n-1} \sum_{j_1=2}^{n} R^{(1)}_{1,j_1} R^{(2)}_{j_1-1,j_2} R^{(3)}_{j_2-1,j_3} \cdots R_{j_{n-2}-1,2}, \tag{2.42}$$

where $j_{n-1} = 2$ and the matrices $R^{(k)}$ are given by (2.9), (2.10), (2.11), and (2.12). All other elements of $Q^{(n)}$ can be derived from this single element. Elements of the first row are given by

$$Q^{(n)}_{1,n-1} = \frac{\partial Q^{(n)}_{1n}}{\partial \theta_{p(n,n-1)}}, \tag{2.43}$$

$$Q^{(n)}_{1l} = \frac{\partial \left(\mathcal{D}^{(n)}_{1l}\right)}{\partial \theta_{p(n,l)}}, \quad l = 1,2,\ldots,n-2, \tag{2.44}$$

where $\mathcal{D}^{(n)}_{1l}$ = Coefficient of $\prod_{m=l+1}^{n-1} \cos\theta_{p(n,m)}$ in $Q^{(n)}_{1n}$. Elements of the second row are given by

$$Q^{(n)}_{2l} = \frac{\partial Q^{(n)}_{1l}}{\partial \theta_1}, \quad l = 1,2,\ldots,n. \tag{2.45}$$

Elements of the remaining rows are given by

$$Q_{il}^{(n)} = \frac{\partial \mathcal{B}_{il}^{(n)}}{\partial \theta_{i-1}}, \quad i = 3,4,\ldots,n;\; l = 1,2,\ldots,n, \tag{2.46}$$

where $\mathcal{B}_{il}^{(n)}$ = *Coefficient of* $\prod_{r=1}^{i-2} \cos\theta_r$ *in* $Q_{1l}^{(n)}$.

3. Example: SO(3)**.** We will now derive the SO(3) matrix using Theorem 2.7. We will first get the expression for $Q_{13}^{(3)}$ (see (2.42)):

$$Q_{13}^{(3)} = R_{12}^{(1)} R_{12}^{(2)} + R_{13}^{(1)} R_{22}^{(2)}. \tag{3.1}$$

From (2.9) and (2.10), we have

$$R_{12}^{(1)} = \sin\theta_1, \qquad R_{13}^{(1)} = \cos\theta_1 \sin\theta_2. \tag{3.2}$$

From (2.9) and (2.11), we get

$$R_{12}^{(2)} = \sin\theta_3, \qquad R_{22}^{(2)} = \cos\theta_3. \tag{3.3}$$

Therefore, we obtain

$$Q_{13}^{(3)} = \sin\theta_1 \sin\theta_3 + \cos\theta_1 \sin\theta_2 \cos\theta_3. \tag{3.4}$$

From (2.43), $Q_{12}^{(3)}$ is given as

$$Q_{12}^{(3)} = \frac{\partial Q_{13}^{(3)}}{\partial \theta_3} = \sin\theta_1 \cos\theta_3 - \cos\theta_1 \sin\theta_2 \sin\theta_3, \tag{3.5}$$

and from (2.44), $Q_{11}^{(3)}$ is given as

$$Q_{11}^{(3)} = \frac{\partial \mathcal{D}_{11}^{(3)}}{\partial \theta_2}, \tag{3.6}$$

where $\mathcal{D}_{11}^{(3)}$ = Coefficient of $\prod_{m=2}^{2} \cos\theta_{p(3,m)}$ in $Q_{13}^{(3)}$. Thus,

$$Q_{11}^{(3)} = \cos\theta_1 \cos\theta_2. \tag{3.7}$$

The second row of $Q^{(3)}$ is given by (2.45):

$$Q_{2l}^{(3)} = \frac{\partial Q_{1l}^{(3)}}{\partial \theta_1}, \quad l = 1,2,3. \tag{3.8}$$

Therefore,

$$\begin{aligned} Q_{21}^{(3)} &= -\sin\theta_1 \cos\theta_2, \\ Q_{22}^{(3)} &= \cos\theta_1 \cos\theta_3 + \sin\theta_1 \sin\theta_2 \sin\theta_3, \\ Q_{23}^{(3)} &= \cos\theta_1 \sin\theta_3 - \sin\theta_1 \sin\theta_2 \cos\theta_3. \end{aligned} \tag{3.9}$$

The last row is given by (2.46):

$$Q_{3l}^{(3)} = \frac{\partial \mathcal{B}_{3l}^{(3)}}{\partial \theta_2}, \quad l = 1, 2, 3, \tag{3.10}$$

where $\mathcal{B}_{3l}^{(3)}$ = Coefficient of $\prod_{r=1}^{1} \cos\theta_r$ in $Q_{1l}^{(3)}$. Therefore, we have

$$\begin{aligned} Q_{31}^{(3)} &= -\sin\theta_2, \\ Q_{32}^{(3)} &= -\cos\theta_2 \sin\theta_3, \\ Q_{33}^{(3)} &= \cos\theta_2 \cos\theta_3. \end{aligned} \tag{3.11}$$

The $Q^{(3)}$ matrix that we have derived agrees with the standard representation as expected.

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