

# Efficient calculation of nematic singular potential

Lucas Myers

April 9, 2024

## 1 Problem statement

Given a traceless, symmetric tensor  $Q$  whose eigenvalues  $\lambda_i$  satisfy:

$$-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3} \quad (1)$$

we seek to invert the following function of  $Q$  for a traceless, symmetric tensor  $\Lambda$ :

$$Q = \frac{1}{Z[\Lambda]} \int_{S^2} (\mathbf{p} \otimes \mathbf{p} - \frac{1}{3}I) \exp(\mathbf{p}^T \Lambda \mathbf{p}) dS(\mathbf{p}) \quad (2)$$

with

$$Z[\Lambda] = \int_{S^2} \exp(\mathbf{p}^T \Lambda \mathbf{p}) dS(\mathbf{p}) \quad (3)$$

In addition to calculating the value of  $\Lambda$ , we also seek the value of the Jacobian of the transformation for use in solving implicit time-stepping equations for  $Q$ . The inversion and calculation of the Jacobian can be done in a straightforward way using a Newton-Rhapson method. However, it is also true that  $Q$  and  $\Lambda$  are simultaneously diagonalized. That is, given some  $R \in SO(3)$  for which:

$$R^T Q R = \text{diag}(\lambda_1, \lambda_2, \lambda_3) \quad (4)$$

we also have that  $R^T \Lambda R$  is diagonal. We may leverage this fact in order to make the inversion significantly more efficient, which will be the goal of this note.

## 2 Mapping to different bases

Call the space of traceless, symmetric tensors  $S^{TR}$ . Because  $Q, \Lambda \in S^{TR}$ , we may represent them using five degrees of freedom. For concreteness, define them as:

$$Q = \begin{bmatrix} Q_1 & Q_2 & Q_3 \\ Q_2 & Q_4 & Q_5 \\ Q_3 & Q_5 & -(Q_1 + Q_4) \end{bmatrix} \quad (5)$$

and call the mapping  $\phi : S^{TR} \rightarrow \mathbb{R}^5$  the mapping which sends a traceless, symmetric tensor to its degrees of freedom. Additionally, call  $A : S^{TR} \rightarrow S^{TR}$  the function which inverts eq. (2). Further, since  $Q, \Lambda \in S^{TR}$  are simultaneously diagonalizable, we have a mapping  $\text{diag} : S^{TR} \rightarrow D^{TR} \times SO(3)$  which sends each tensor to the space of diagonal, traceless, symmetric tensors  $D^{TR}$  crossed with the set of orientation-preserving rotation matrices  $SO(3)$ . We may also represent an element of  $D^{TR} \times SO(3)$  in terms of two eigenvalues, and the columns associated with the rotation matrix (which is some subspace of  $\mathbb{R}^9$ ). Call the mapping  $\psi$ . Finally, call  $a$  the mapping from the degrees

of freedom of  $Q$  to the degrees of freedom of  $\Lambda$ . Given all this, we may construct the following commutative diagram:

$$\begin{array}{ccccc}
& D^{Tr} \times SO(3) & \xrightarrow{A|_{D^{Tr} \times I}} & D^{Tr} \times SO(3) & \\
\text{diag} \nearrow & \downarrow \psi & & \downarrow \psi & \searrow \text{diag} \\
S^{Tr} & \xrightarrow{A} & S^{Tr} & & \\
\downarrow \phi & & \downarrow \phi & & \\
& \mathbb{R}^2 \times \mathbb{R}^9 & \xrightarrow{a|_{\mathbb{R}^2} \times I} & \mathbb{R}^2 \times \mathbb{R}^9 & \\
& \downarrow \phi & & \downarrow \phi & \\
\mathbb{R}^5 & \xrightarrow{a} & \mathbb{R}^5 & & 
\end{array}$$

Given this, we may decompose  $a$  as:

$$a = (\phi \circ \text{diag}^{-1} \circ \psi^{-1}) \circ (a|_{\mathbb{R}^2} \times I) \circ (\psi \circ \text{diag} \circ \phi^{-1}) \quad (6)$$

The Jacobian of the mapping is then:

$$da = [d(\phi \circ \text{diag}^{-1} \circ \psi^{-1})] [d(a|_{\mathbb{R}^2} \times I)] [d(\psi \circ \text{diag} \circ \phi^{-1})] \quad (7)$$

where each quantity in brackets is a matrix.

Note that  $(\psi \circ \text{diag} \circ \phi^{-1})$  may be calculated efficiently by any eigenvalue algorithm, and that  $(\phi \circ \text{diag}^{-1} \circ \psi^{-1})$  may be calculated efficiently by two matrix multiplications (by the corresponding rotation matrix). The  $a|_{\mathbb{R}^2}$  mapping may also be efficiently calculated, given that the Newton-Rhaphson inversion method happens in a subspace – this reduces the number of numerical quadrature operations by a factor of 10, and the added symmetry of the integrands allows us to integrate over only one octant of the sphere which reduces the number of quadrature points by a factor of approximately eight.

The  $d(a|_{\mathbb{R}^2})$  mapping falls out of the Newton-Rhaphson calculation on the subspace, but the other calculations involving the diagonalization process are less straightforward. In particular, the diagonalization mapping is not locally invertible in the case of repeated eigenvalues. In this case, eigenvectors corresponding to repeated eigenvalues form a plane in  $\mathbb{R}^3$  and the rotation matrix  $R$  which diagonalizes  $Q$  can be rotated continuously in that plane to give another rotation matrix which diagonalizes  $Q$ . We will deal with this situation by perturbing repeated eigenvalues, and then taking the perturbation to zero once all of the compositions have been done. The rest of this note is concerned with calculating the derivatives of each of the diagonalization and inverse diagonalization mappings.

### 3 Derivative of the diagonalization mapping

This calculation depends on the fact that, even though we may not write down an explicit expression for the calculation of the eigenvalues and eigenvectors of a  $3 \times 3$  matrix, if the matrix depends on some parameter  $t$ , we may write down derivatives of the eigenvalues and eigenvectors with respect to  $t$  in terms of the matrix, its eigenvalues, and its eigenvectors. The motivation for this calculation is given in this MathOverflow post.

In short, suppose  $Q$  is parameterized by some value  $t$ . Then:

$$\dot{\lambda}_i = \langle \dot{Q} \mathbf{n}_i, \mathbf{n}_i \rangle \quad (8)$$

where  $\dot{\lambda}_i$  is the derivative of  $\lambda_i$  with respect to  $t$ ,  $\dot{Q}$  is the derivative of  $Q$  with respect to  $t$ ,  $\mathbf{n}_i$  is the eigenvector corresponding to  $\lambda_i$ , and  $\langle, \rangle$  is the usual inner product. Additionally, we may calculate:

$$\dot{\mathbf{n}}_i = \sum_{i \neq j} \frac{1}{\lambda_i - \lambda_j} \langle \dot{Q} \mathbf{n}_i, \mathbf{n}_j \rangle \mathbf{n}_j \quad (9)$$

Call  $dQ$  the  $5 \times 3 \times 3$  tensor which collects the derivatives of  $Q$  with respect to each of its degrees of freedom. Then we may define  $d\lambda_i$  a  $1 \times 5$  tensor which collects derivatives of each  $\lambda_i$  with respect to the degrees of freedom of  $Q$ :

$$d\lambda_i = \langle dQ \mathbf{n}_i, \mathbf{n}_i \rangle \quad (10)$$

We may also define  $d\mathbf{n}_i$  to be a  $3 \times 5$  tensor which corresponds to derivatives of  $\mathbf{n}_i$  with respect to each degree of freedom of  $Q$ :

$$d\mathbf{n}_i = \sum_{i \neq j} \frac{1}{\lambda_i - \lambda_j} \mathbf{n}_j \langle dQ \mathbf{n}_i, \mathbf{n}_j \rangle \quad (11)$$

When we come to handling the case of repeated eigenvalues we will need to separate out the eigenvalue factors from our calculations. To this end, we define a collection of nine scalars indexed by  $i$  and  $j$ :

$$\gamma_{ij} = \frac{1}{\lambda_i - \lambda_j} \quad (12)$$

Further, for notational simplicity, we define a corresponding collection of nine  $3 \times 5$  matrices indexed by  $i$  and  $j$  as:

$$S_{ij} = \mathbf{n}_j \langle dQ \mathbf{n}_i, \mathbf{n}_j \rangle \quad (13)$$

Finally, we write out the  $11 \times 5$  Jacobian of the diagonalization as:

$$J = \begin{bmatrix} d\lambda \\ d\mathbf{n} \end{bmatrix} \quad (14)$$

with

$$d\lambda = \begin{bmatrix} d\lambda_1 \\ d\lambda_2 \end{bmatrix} \quad (15)$$

Note that we are uninterested in  $\lambda_3$  because  $Q$  is traceless, and so  $\lambda_3 = -(\lambda_1 + \lambda_2)$ . Additionally,

$$d\mathbf{n} = \begin{bmatrix} d\mathbf{n}_1 \\ d\mathbf{n}_2 \\ d\mathbf{n}_3 \end{bmatrix} \quad (16)$$

## 4 Reduced singular potential derivative

Here since  $a|_{\mathbb{R}^2}$  is a map from  $\mathbb{R}^2$  to  $\mathbb{R}^2$ , its derivative is a  $2 \times 2$  matrix. Notate it:

$$da = \begin{bmatrix} da_{11} & da_{12} \\ da_{21} & da_{22} \end{bmatrix} \quad (17)$$

This is calculated in the course of numerically calculating  $a|_{\mathbb{R}^2}$ . The Jacobian of  $a|_{\mathbb{R}^2} \times I$  is then given by:

$$K = \begin{bmatrix} da & 0_{2 \times 9} \\ 0_{9 \times 2} & I_{9 \times 9} \end{bmatrix} \quad (18)$$

where we have notated the dimensions of each of the block matrices.

## 5 Derivative of rotation back to original basis

This mapping maps  $(a_1, a_2)$  – the eigenvalues of the matrix  $\Lambda$  – and all the entries of the rotation matrix – which are exactly the eigenvectors – back to the degrees of freedom of a generic traceless, symmetric tensor. Explicitly the mapping is given by:

$$R\Lambda R^T = \begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 & \mathbf{n}_3 \end{bmatrix} \begin{bmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & -(a_1 + a_2) \end{bmatrix} \begin{bmatrix} \mathbf{n}_1^T \\ \mathbf{n}_2^T \\ \mathbf{n}_3^T \end{bmatrix} \quad (19)$$

Multiplying this out explicitly yields:

$$R\Lambda R^T = a_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + a_2 \mathbf{n}_2 \otimes \mathbf{n}_2 - (a_1 + a_2) \mathbf{n}_3 \otimes \mathbf{n}_3 \quad (20)$$

The final vector in  $\mathbb{R}^5$  associated with this mapping is the associated degrees of freedom (see eq. (5)). The derivative of the mapping is a  $5 \times 11$  matrix where the rows are indexed by which degree of freedom is being mapped to, and the columns respectively correspond to derivatives with respect to:  $a_1$  and  $a_2$ , and then each of the entries of the three eigenvectors. To notate this appropriately, define  $V$  to be a  $5 \times 3 \times 3$  tensor which is a collection of five  $3 \times 3$  matrices which have a 1 in the first entry where a degree of freedom shows up, and a zero everywhere else. Explicitly:

$$V = \left[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \right] \quad (21)$$

Then  $V : (R\Lambda R^T)$  is a collection of the five degrees of freedom associated with  $(R\Lambda R^T)$ , where  $:$  is a contraction over the two inner indices. To get the Jacobian, we just take derivatives with respect to appropriate parameters. Define a set of three  $5 \times 3$  matrices:

$$T_i = \frac{d(V : (\mathbf{n}_i \otimes \mathbf{n}_i))}{d\mathbf{n}_i} \quad (22)$$

where the column index corresponds to which element of  $\mathbf{n}_i$  the derivative is being taken with respect to. We may also write the derivative with respect to the  $a_i$  as:

$$dF_i = V : (\mathbf{n}_i \otimes \mathbf{n}_i) \quad (23)$$

Thus, the Jacobian of this rotation mapping is given by:

$$L = \begin{bmatrix} dF & dR \end{bmatrix} \quad (24)$$

where

$$dF = \begin{bmatrix} dF_1 & dF_2 \end{bmatrix} \quad (25)$$

and

$$dR = \begin{bmatrix} a_1 T_1 & a_2 T_2 & -(a_1 + a_2) T_3 \end{bmatrix} \quad (26)$$

## 6 Explicit expression of Jacobian for non-degenerate eigenvalues

The derivative of the composition of these mappings is just the product of derivatives:

$$\begin{aligned} LKJ &= \begin{bmatrix} dF & dR \end{bmatrix} \begin{bmatrix} da & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} d\lambda \\ d\mathbf{n} \end{bmatrix} \\ &= dF da d\lambda + dR d\mathbf{n} \\ &= dF da d\lambda + a_1 T_1 (\gamma_{12} S_{12} + \gamma_{13} S_{13}) \\ &\quad + a_2 T_2 (\gamma_{21} S_{21} + \gamma_{23} S_{23}) \\ &\quad - (a_1 + a_2) T_3 (\gamma_{31} S_{31} + \gamma_{32} S_{32}) \end{aligned} \quad (27)$$

We may simplify this expression by noting that  $\gamma_{ij} = -\gamma_{ji}$ , and that:

$$T_i S_{ij} = T_j S_{ji} \quad (28)$$

for  $i \neq j$ . To see this, we must explicitly write out both matrices:

$$T_i S_{ij} = \frac{d(V : (\mathbf{n}_i \otimes \mathbf{n}_i))}{d\mathbf{n}_i} \mathbf{n}_j \langle dQ \mathbf{n}_i, \mathbf{n}_j \rangle \quad (29)$$

But note that:

$$\langle dQ \mathbf{n}_i, \mathbf{n}_j \rangle = \langle dQ \mathbf{n}_j, \mathbf{n}_i \rangle \quad (30)$$

because  $dQ$  is symmetric for all indices. Additionally, by treating each eigenvalue as a column in a rotation matrix, and summing over repeated Greek (but not Latin!) indices, we may calculate the following:

$$\begin{aligned} \frac{d(V : (\mathbf{n}_i \otimes \mathbf{n}_i))}{d\mathbf{n}_i} \mathbf{n}_j &= \frac{\partial (V_{\mu\nu} R_{\mu i} R_{\nu i})}{\partial R_{\sigma i}} R_{\sigma j} \\ &= V_{\mu\nu} (R_{\mu i} \delta_{\nu\sigma} + R_{\nu i} \delta_{\sigma\mu}) R_{\sigma j} \\ &= V_{\mu\nu} (R_{\mu i} R_{\nu j} + R_{\nu i} R_{\mu j}) \\ &= \frac{d(V : (\mathbf{n}_j \otimes \mathbf{n}_j))}{d\mathbf{n}_j} \mathbf{n}_i \end{aligned} \quad (31)$$

where, for the last equality we have noted that the expression is symmetric in  $i$  and  $j$ . Invoking these two identities we may write:

$$\begin{aligned} LKJ &= dF da d\lambda + (a_1 - a_2) \gamma_{12} T_1 S_{12} \\ &\quad + (2a_1 + a_2) \gamma_{13} T_1 S_{13} \\ &\quad + (a_1 + 2a_2) \gamma_{23} T_2 S_{23} \end{aligned} \quad (32)$$

## 7 Explicit expression of Jacobian for nearly degenerate eigenvalues

As stated above, the mapping from a traceless, symmetric tensor to its eigenvalues and eigenvectors is not uniquely defined locally in the case of repeated eigenvalues. Indeed, as the eigenvalues approach each other the  $\gamma_{ij}$  factors tend towards infinity. To make analytic progress on this issue, we consider a set of eigenvalues which is slightly perturbed from being degenerate. Define:

$$Q_0 = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & -2\lambda \end{bmatrix} \quad (33)$$

and

$$Q = Q_0 + \begin{bmatrix} \epsilon & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\epsilon \end{bmatrix} \quad (34)$$

where  $\epsilon$  is a small perturbation. Then we may Taylor expand the eigenvalues of the singular potential as:

$$a_i(Q) = a_i(Q_0) + \epsilon da_{1i} + \mathcal{O}(\epsilon^2) \quad (35)$$

Note that  $\Lambda$  also has repeated eigenvalues because, since  $Q$  and  $\Lambda$  are simultaneously diagonalized and  $Q$  remains diagonalized by a rotation in the plane of its eigenvectors,  $\Lambda$  must also remain

diagonalized under such a transformation. Hence,  $a_i(Q_0) = a_1$  for any  $i$  and some fixed  $a_1$ . In this case, the expression reduces to:

$$\begin{aligned}
LKJ = & dF da d\lambda + (da_{11} - da_{12}) T_1 S_{12} \\
& + (3a_1 + \epsilon(2da_{11} + da_{12})) \frac{1}{3\lambda} T_1 S_{13} \\
& + (3a_1 + \epsilon(da_{11} + 2da_{12})) \frac{1}{3\lambda - \epsilon} T_2 S_{23}
\end{aligned} \tag{36}$$

This is a perfectly analytic function, even as  $\epsilon \rightarrow 0$ . The only problem that we might have is if  $\lambda \rightarrow 0$ . In this case, we may explicitly calculate the singular potential and the corresponding Jacobian – indeed, the singular potential just takes on all zero values when  $Q$  does.

## 8 Inverting the reduced singular potential

In this case, Eq. (2) reduces to two degrees of freedom. We may write this explicitly as:

$$Q_0 = \frac{1}{Z} \int_{S^2} (x^2 - \frac{1}{3}) \exp [x^2 (2\Lambda_0 + \Lambda_1) + y^2 (\Lambda_0 + 2\Lambda_1) - (\Lambda_0 + \Lambda_1)] \tag{37}$$

$$Q_1 = \frac{1}{Z} \int_{S^2} (y^2 - \frac{1}{3}) \exp [x^2 (2\Lambda_0 + \Lambda_1) + y^2 (\Lambda_0 + 2\Lambda_1) - (\Lambda_0 + \Lambda_1)] \tag{38}$$

where we have used that

$$x^2 \Lambda_0 + y^2 \Lambda_1 - z^2 (\Lambda_0 + \Lambda_1) = x^2 (2\Lambda_0 + \Lambda_1) + y^2 (\Lambda_0 + 2\Lambda_1) - (\Lambda_0 + \Lambda_1) \tag{39}$$