Efficient calculation of nematic singular potential

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1 Eigenvalue and eigenvector derivatives

To begin, we list formulas for the derivatives of eigenvalues and eigenvectors of a matrix in terms of the original matrix and the corresponding values:

$$\dot{\lambda}_i = \left\langle \dot{B} n_i, n_i \right\rangle \tag{1}$$

where here the overdot indicates derivative with respect to some variable, i characterizes the eigenvector/eigenvalue pair, B is the matrix whose eigenvalues we are considering, and $\langle , \rangle$ denotes the inner product. The derivative of the eigenvectors is:

$$\dot{n}_i = \sum_{i \neq j} \frac{1}{\lambda_i - \lambda_j} \left\langle \dot{B} n_i, n_j \right\rangle n_j \tag{2}$$

For sake of compactness, we define dB to be a $5 \times 3 \times 3$ tensor where the first entry denotes which degree of freedom of a traceless symmetric tensor the derivative is being taken with respect to. Then each eigenvector derivative can be thought of as a 3×5 matrix and written as:

$$dn_i = \sum_{i \neq j} \frac{1}{\lambda_i - \lambda_j} n_j \left\langle dB\, n_i, n_j \right\rangle \tag{3}$$

Introducing more notation, we may define a collection of 3×5 matrices S_{ij} which correspond to the terms in the sum needed to compute each eigenvector derivative. These are given as:

$$S_{ij} = n_j \left\langle dB\, n_i, n_j \right\rangle \tag{4}$$

Finally, to capture the coefficients we introduce some scalars γ_{ij} as:

$$\gamma_{ij} = \frac{1}{\lambda_i - \lambda_j} \tag{5}$$

Note that $\gamma_{ij} = -\gamma_{ji}$. Finally, we rewrite the eigenvalue derivatives in the same way, as 1×5 vectors:

$$d\lambda_i = \left\langle dB\, n_i, n_i \right\rangle \tag{6}$$

Then the Jacobian matrix J of the mapping which brings a traceless, symmetric tensor to its eigenvalues and eigenvectors can be written as:

$$J = \begin{bmatrix} d\lambda \\ dn \end{bmatrix} \tag{7}$$

where:

$$d\lambda = \begin{bmatrix} d\lambda_1 \\ d\lambda_2 \end{bmatrix} \tag{8}$$

and

$$dn = \begin{bmatrix} dn_1 \\ dn_2 \\ dn_3 \end{bmatrix} \tag{9}$$

2 Diagonal singular potential derivative

In an eigenbasis which diagonalizes Q (and thus diagonalizes $\Lambda(Q)$), the mapping Λ is a map from $\mathbb{R}^2 \to \mathbb{R}^2$. Hence, the Jacobian is a 2×2 matrix:

$$d\Lambda = \begin{bmatrix} d\Lambda_{11} & d\Lambda 12 \\ d\Lambda 21 & d\Lambda 22 \end{bmatrix} \tag{10}$$

The mapping from rotation matrices to rotation matrices is just the identity for this, so the total Jacobian of this transformation K is given by:

$$K = \begin{bmatrix} d\Lambda & 0_{2\times 9} \\ 0_{9\times 2} & I_{9\times 9} \end{bmatrix} \tag{11}$$

where we have indicated the dimensions associated with the zero and identity matrices.

3 Derivative of rotation back to original basis

This mapping maps (Λ_1, Λ_2) and all of the entries of the rotation matrix back to the degrees of freedom of a generic traceless, symmetric tensor via the mapping:

$$R\Lambda R^T = \begin{bmatrix} n_1 & n_2 & n_3 \end{bmatrix} \begin{bmatrix} \Lambda_1 & 0 & 0 \\ 0 & \Lambda_2 & 0 \\ 0 & 0 & -(\Lambda_1 + \Lambda_2) \end{bmatrix} \begin{bmatrix} n_1^T \\ n_2^T \\ n_3^T \end{bmatrix} \tag{12}$$

since the eigenvectors are just the columns of the rotation matrix. Multiplying this out yields:

$$R\Lambda R^T = \Lambda_1 \, n_1 \otimes n_1 + \Lambda_2 \, n_2 \otimes n_2 - (\Lambda_1 + \Lambda_2) \, n_3 \otimes n_3 \tag{13}$$

The final vector of the mapping is just the degrees of freedom of this traceless, symmetric matrix. The derivative of this mapping is a 5×11 matrix where the first two columns are derivatives with respect to Λ_1 and Λ_2, and the last nine are derivatives with respect to each entry of the rotation matrix.

Define V to be a $5 \times 3 \times 3$ symmetric tensor to be a collection of matrices that have a one in the place of each of the degrees of freedom (corresponding to the first index) and zeros everywhere else. Then we may define a set of 5×3 matrices:

$$T_i = \frac{d\big(V : (n_i \otimes n_i)\big)}{dn_i} \tag{14}$$

where the column index corresponds to which element of n_i the derivative is being taken with respect to. Additionally, we may rewrite the derivatives with respect to Λ_i as:

$$dF_i = V : (n_i \otimes n_i) \tag{15}$$

Thus, the derivative of the final transformation may be written as:

$$L = \begin{bmatrix} dF & dR \end{bmatrix} \tag{16}$$

where we have defined:

$$dF = \begin{bmatrix} dF_1 & dF_2 \end{bmatrix} \tag{17}$$

and

$$dR = \begin{bmatrix} \Lambda_1 T_1 & \Lambda_2 T_2 & -(\Lambda_1 + \Lambda_2) T_3 \end{bmatrix} \tag{18}$$

4 Forumla for non-degenerate eigenvalues

To find the derivative of the composition, we just have to multiply all of the derivatives:

$$\begin{aligned} LKJ &= \begin{bmatrix} dF & dR \end{bmatrix} \begin{bmatrix} d\Lambda & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} d\lambda \\ dn \end{bmatrix} \\ &= dF\, d\Lambda\, d\lambda + dR\, dn \\ &= dF\, d\Lambda\, d\lambda + \Lambda_1 T_1 \left(\gamma_{12} S_{12} + \gamma_{13} S_{13}\right) \\ &\qquad + \Lambda_2 T_2 \left(-\gamma_{12} S_{21} + \gamma_{23} S_{23}\right) \\ &\qquad + (\Lambda_1 + \Lambda_2) T_3 \left(\gamma_{13} S_{31} + \gamma_{23} S_{32}\right) \end{aligned} \tag{19}$$

We may simplify this by recognizing that:

$$T_i S_{ij} = T_j S_{ji} \tag{20}$$

for $i \neq j$. We may see this by writing out explicitly in terms of definitions:

$$T_i S_{ij} = \frac{d\big(V : (n_i \otimes n_i)\big)}{dn_i} n_j \left\langle dB\, n_i, n_j \right\rangle \tag{21}$$

Now note that:

$$\left\langle dB\, n_i, n_j \right\rangle = \left\langle dB\, n_j, n_i \right\rangle \tag{22}$$

since dB is symmetric for all indices. Additionally, by treating each eigenvector as a column of the rotation matrix and summing over repeated Greek indices (but not Latin indices), we may calculate the following:

$$\begin{aligned} \frac{d\big(V : (n_i \otimes n_i)\big)}{dn_i} n_j &= \frac{\partial\big(V_{\mu\nu} R_{\mu i} R_{\nu i}\big)}{\partial R_{\sigma i}} R_{\sigma j} \\ &= V_{\mu\nu} \left(R_{\mu i} \delta_{\sigma\nu} + R_{\nu i} \delta_{\sigma\mu}\right) R_{\sigma j} \\ &= V_{\mu\nu} \left(R_{\mu i} R_{\nu j} + R_{\nu i} R_{\mu j}\right) \\ &= \frac{d\big(V : (n_j \otimes n_j)\big)}{dn_j} n_i \end{aligned} \tag{23}$$

where for the last equality we notice that the penultimate expression is symmetric in i and j so that the entire expression must be. All told we may write:

$$\begin{aligned} LKJ = dF\, d\Lambda\, d\lambda + &\left(\Lambda_1 - \Lambda_2\right) \gamma_{12} T_1 S_{12} \\ &+ \left(2\Lambda_1 + \Lambda_2\right) \gamma_{13} T_1 S_{13} \\ &+ \left(\Lambda_1 + 2\Lambda_2\right) \gamma_{23} T_2 S_{23} \end{aligned} \tag{24}$$

A pretty compact expression, all told. The matrices involved are also reasonably easy to calculate.

5 Formula for (nearly) degenerate eigenvalues

If the eigenvalues of Q, λ_1 and λ_2 become such that they are *almost* equal, to the point where γ_{12} diverges, then our diagonalized, nearly degenerate Q-tensor may be written as:

$$Q = \mathrm{diag}(\lambda_1 + \varepsilon, \lambda_1, -2\lambda - \varepsilon) \tag{25}$$

with ε a small perturbation. Note that Q is still traceless and symmetric in this case. Supposing that ε is small, we may Taylor expand the reduced singular potential as:

$$\Lambda_i(Q) \approx \Lambda_i(Q_0) + \varepsilon d\Lambda_{1i} \tag{26}$$

Note that, because Q and Λ are simulataneously diagonalized, it follows that when Q has degenerate eigenvalues, Λ must as well, otherwise a rotation in the plane spanned by the eigenvectors of degenerate eigenvalues of Q would make Λ not diagonal. Hence, $\Lambda_i(Q_0) = \Lambda_1$ for some Λ_1. In this case, the formula reduces to:

$$\begin{aligned} LKJ = dF\, d\Lambda\, d\lambda + &\left(d\Lambda_{11} - d\Lambda_{12}\right) T_1 S_{12} \\ &+ \left(3\Lambda_1 + \varepsilon\left(2d\Lambda_{11} + d\Lambda_{12}\right)\right) \gamma_{13} T_1 S_{13} \\ &+ \left(3\Lambda_1 + \varepsilon\left(d\Lambda_{11} + 2d\Lambda_{12}\right)\right) \gamma_{23} T_2 S_{23} \end{aligned} \tag{27}$$

Indeed, everything here is nonsingular so this formula works perfectly well