Calculation of Response Matrices

Let the (vector) response due to an applied external force f be

$$\delta \mathbf{a} = \mathbf{A}\mathbf{f} \qquad (1)$$

where we can consider, respectively, the responses in force, conformation, and energy using:

$$\begin{aligned} \mathbf{A} &= \mathbf{I} : \mathbf{a} = \mathbf{f} \\ \mathbf{A} &= \mathbf{C} : \mathbf{a} = \mathbf{r} \\ \mathbf{A} &= \mathbf{C}^{1/2} : \mathbf{a} = \mathbf{e} \end{aligned} \qquad \textbf{(2)}1$$

Warning:

Note that:

$$\mathbf{C}^{1/2} = \sum_n \frac{1}{\sqrt{\lambda_n}} \mathbf{u}_n \mathbf{u}_n^T = \mathbf{U}\Lambda^{-1/2}\mathbf{U}^T \qquad (3)$$

where λ_n are the eigenvalues of K, $\mathbf{u}_n$ the corresponding eigenvectors:

$$\mathbf{U}^T \mathbf{K} \mathbf{U} = \Lambda \qquad (4)$$

Perturbing a contact

For the case of a force of magnitude f^{kl} along contact k-l the "vector response" at site i is:

$$\delta \mathbf{a}_i^{kl} = \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)\hat{\mathbf{d}}_{kl} f^{kl} \qquad (5)$$

The scalar response is:

$$R_i^{kl} = \left\|\delta \mathbf{a}_i^{kl}\right\|^2 = \left(f^{kl}\right)^2 \hat{\mathbf{d}}_{kl}^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)\hat{\mathbf{d}}_{kl} \qquad (6)$$

Thus, if we average over several instances of forcing the kl contact and using arbitrarily $\left\langle \left(f^{kl}\right)^2 \right\rangle = 1$, we get:

$$R_i^{kl} = \hat{\mathbf{d}}_{kl}^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)\hat{\mathbf{d}}_{kl} \qquad (7)$$

Mutating a site

The mutation of site l is modeled with:

$$\mathbf{f}^l = \sum_{k \sim l} \mathbf{f}^{kl} \qquad (8)$$

where the sum is over sites k in contact with the mutated site l. The response at site i due to this mutation is given by

$$\delta \mathbf{a}_i^l = \sum_{k \sim l} \delta \mathbf{a}_i^{kl} = \sum_{k \sim l} \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)\hat{\mathbf{d}}_{kl} f^{kl} \qquad (9)$$

The scalar response, averaged over independent mutations at the same site l is:

$$R_i^l = \left\|\delta \mathbf{a}_i^l\right\|^2 = \sum_{k \sim l} \sum_{k' \sim l} \delta \mathbf{a}_i^{kl} . \delta \mathbf{a}_i^{k'l} = \sum_{k \sim l} \sum_{k' \sim l} \left\langle f^{kl} f^{k'l} \right\rangle \hat{\mathbf{d}}_{kl}^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik'}\right)\hat{\mathbf{d}}_{k'l} \qquad (10)$$

Case of independent forces

For the case in which we pick the forces along the different contacts of l INDEPENDENTLY:

$$\left\langle f^{kl} f^{k'l} \right\rangle = \left\langle (f^{kl})^2 \right\rangle \delta_{kk'} \tag{11}$$

If we use the same distribution to pick forces for all contacts (i.e. the average does not depend on kl) then we can, without loss of generality, use

$$\left\langle f^{kl} f^{k'l} \right\rangle = \delta_{kk'} \tag{12}$$

Replacing (12) into (10) we find:

$$R_i^l = \sum_{k\sim l} \hat{\mathbf{d}}_{kl}^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right)^T \left(\mathbf{A}_{il} - \mathbf{A}_{ik}\right) \hat{\mathbf{d}}_{kl} \tag{13}$$

Thus, the "magic formula" to calculate the response matrices is (13), where A is either the identity matrix, for the force, the covariance matrix, for the response in structure, and the square root of the covariance matrix, for the response in energy.