1 DG Error function

For a given set of N particles with positions $\vec{r}_i$, the distance geometry error function is given as:

$$
\begin{aligned}
\operatorname{errf}(\{\vec{r}_i\}) = & \underbrace{\sum_{i<j}^{N} \left[\max^2\left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1\right) + \max^2\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + (\vec{r}_j - \vec{r}_i)^2} - 1\right)\right]}_{\text{Distance errors}} \\
& + \underbrace{\sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} \left[\max^2\left(0, V_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) - U_V\right) + \max^2\left(0, L_V - V_{\alpha\beta\gamma\delta}(\{\vec{r}_i\})\right)\right]}_{\text{Chiral errors}} \\
& + \underbrace{\sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_\phi, L_\phi) \in D} \max^2\left(0, \left|\phi_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) + \begin{cases} 2\pi & \phi < \frac{U_\phi + L_\phi - 2\pi}{2} \\ 0 & \\ -2\pi & \phi > \frac{U_\phi + L_\phi + 2\pi}{2} \end{cases} - \frac{U_\phi + L_\phi}{2}\right| - \frac{U_\phi - L_\phi}{2}\right)}_{\text{Dihedral errors}}.
\end{aligned}
\tag{1}
$$

Within the distance errors, the symbols U_{ij} and L_{ij} are the upper and lower distance bounds for the atoms i and j.

Within the chiral errors, C is a set of chiral constraint tuples consisting of the sets $S_\alpha, S_\beta, S_\gamma$ and S_δ. These contain mutually disjoint particle indices and contain at least one element. In further notation, $\vec{s}$ denotes the average spatial position of all elements of a set, e.g. for S_α:

$$
\vec{s}_\alpha = \frac{1}{|S_\alpha|} \sum_{i=1}^{|S_\alpha|} \vec{r}_{S_{\alpha,i}}, \tag{2}
$$

where $|S_\alpha|$ denotes the number of elements in the set and $S_{\alpha,i}$ is the i-th element in the set.

The constraint tuple further consists of the scalars U_V and L_V, which are upper and lower bounds on the volume spanned by the average positions of the sets S_α, S_β, S_γ and S_δ. This volume is calculated in the symbol $V_{\alpha\beta\gamma\delta}$, which is the signed tetrahedron volume spanned by $\vec{s}_\alpha, \vec{s}_\beta, \vec{s}_\gamma$ and $\vec{s}_\delta$:

$$
V_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) = (\vec{s}_\alpha - \vec{s}_\delta)^T \cdot \left[(\vec{s}_\beta - \vec{s}_\delta) \times (\vec{s}_\gamma - \vec{s}_\delta)\right]. \tag{3}
$$

It is important to note that tetrahedron volumes such as U_V are signed values. On odd permutations of indices, these quantities change sign.

Within the dihedral errors, D is a set of dihedral constraint tuples. Each tuple consists of particle index sets $S_\alpha, S_\beta, S_\gamma$ and S_δ. Exactly as for chiral errors, these sets do not intersect and each contain at least a single element. Furthermore, U_ϕ and L_ϕ are upper and lower bounds on the dihedral angle ϕ defined by the particle index sets:

$$
\begin{aligned}
\phi_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) = \operatorname{atan2}\Big(& \left[(\vec{s}_\beta - \vec{s}_\alpha) \times (\vec{s}_\gamma - \vec{s}_\beta)\right] \times \left[(\vec{s}_\gamma - \vec{s}_\beta) \times (\vec{s}_\delta - \vec{s}_\gamma)\right] \cdot \frac{(\vec{s}_\gamma - \vec{s}_\beta)}{|(\vec{s}_\gamma - \vec{s}_\beta)|} \\
& \left[(\vec{s}_\beta - \vec{s}_\alpha) \times (\vec{s}_\gamma - \vec{s}_\beta)\right] \cdot \left[(\vec{s}_\gamma - \vec{s}_\beta) \times (\vec{s}_\delta - \vec{s}_\gamma)\right] \Big)
\end{aligned}
\tag{4}
$$

Here we have used a three-vector dihedral angle definition and inserted the index set average-position differences that constitute the dihedral angle. Another definition of the dihedral angle with merely the inverse cosine is:

$$
\phi_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) = \arccos \frac{\left[(\vec{s}_\alpha - \vec{s}_\beta) \times (\vec{s}_\beta - \vec{s}_\gamma)\right]\left[(\vec{s}_\beta - \vec{s}_\gamma) \times (\vec{s}_\delta - \vec{s}_\gamma)\right]}{|(\vec{s}_\alpha - \vec{s}_\beta) \times (\vec{s}_\beta - \vec{s}_\gamma)||(\vec{s}_\beta - \vec{s}_\gamma) \times (\vec{s}_\delta - \vec{s}_\gamma)|}, \tag{5}
$$

whose derivatives w.r.t. the constituting position vectors are considerably easier to evaluate.

2 Gradient of the error function

E is scalar-valued, so the columnar gradient of the error function is composed of partial derivatives to the individual position vectors $\vec{r}_i$:

$$\nabla E = \left(\frac{\partial E}{\partial \vec{r}_1}, \frac{\partial E}{\partial \vec{r}_2}, \ldots, \frac{\partial E}{\partial \vec{r}_N} \right)$$

Each individual component $(\partial E / \partial \vec{r}_\xi)$ is a vector whose components are the scalar derivatives:

$$\frac{\partial E}{\partial \vec{r}_\xi} = \begin{pmatrix} \partial E / \partial r_{\xi,x} \\ \partial E / \partial r_{\xi,y} \\ \partial E / \partial r_{\xi,z} \end{pmatrix}$$

We split the problem into the main terms:

$$\begin{aligned} \frac{\partial}{\partial \vec{r}_\xi} \operatorname{errf}(\{\vec{r}_i\}) = & \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \left(\sum_{i<j}^{N} \max^2 \left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 \right) \right)}_{1} + \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \left(\sum_{i<j}^{N} \max^2 \left(0, \frac{2L_{ij}^2}{L_{ij}^2 + (\vec{r}_j - \vec{r}_i)^2} - 1 \right) \right)}_{2} \\ & + \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} \max^2 \left(0, V_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) - U_V \right)}_{3} \\ & + \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} \max^2 \left(0, L_V - V_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) \right)}_{4} \\ & + \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_\phi, L_\phi) \in D} \max^2 \left(0, \left| \phi_{\alpha\beta\gamma\delta}(\{\vec{r}_i\}) + \left\{ \begin{array}{r|l} 2\pi & \phi < \frac{U_\phi + L_\phi - 2\pi}{2} \\ 0 & \\ -2\pi & \phi > \frac{U_\phi + L_\phi + 2\pi}{2} \end{array} \right\} - \frac{U_\phi + L_\phi}{2} \right| - \frac{U_\phi - L_\phi}{2} \right)}_{5}. \end{aligned}$$

2.1 Distance error terms

We begin with 1. We use the chain rule:

$$\frac{\partial}{\partial \vec{r}_\xi} \sum_{i<j}^{N} \max^2 \left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 \right) = 2 \sum_{i<j}^{N} \max \left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 \right) \frac{\partial}{\partial \vec{r}_\xi} \max \left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 \right). \tag{6}$$

If $\xi = i$, then:

$$\frac{\partial}{\partial \vec{r}_i} \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 = -\frac{2}{U_{ij}^2} (\vec{r}_j - \vec{r}_i), \tag{7}$$

and likewise, but positive, for $\xi = j$. Consequently:

$$\frac{\partial}{\partial \vec{r}_\xi} \left(\max \left(0, \frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 \right) \right) = \frac{2}{U_{ij}^2} (\vec{r}_j - \vec{r}_i) \left\{ \begin{array}{r|c} -1 & \xi = i \\ 1 & \xi = j \\ 0 & \text{else} \end{array} \right\} = \frac{2}{U_{ij}^2} (\vec{r}_j - \vec{r}_i) (\delta_{\xi j} - \delta_{\xi i}), \tag{8}$$

where we have discarded the possibility of $\frac{(\vec{r}_j - \vec{r}_i)^2}{U_{ij}^2} - 1 < 0$ since this case is adequately covered by the first maximum function. δ is the Kronecker delta. So, in total:

$$
\textcircled{1} = \sum_{i<j}^{N} \left(\delta_{\xi j} - \delta_{\xi i}\right) \underbrace{\frac{4}{U_{ij}^2} \left(\vec{r}_j - \vec{r}_i\right) \max\left(0, \frac{\left(\vec{r}_j - \vec{r}_i\right)^2}{U_{ij}^2} - 1\right)}_{f(i,j)} \tag{9}
$$

We can transform the summation further with Kronecker deltas:

$$
\begin{aligned}
\sum_{i<j}^{N} \left(\delta_{\xi j} - \delta_{\xi i}\right) f(i,j) &= \sum_{i=1}^{\xi-1} f(i,\xi) - \sum_{j=\xi+1}^{N} f(\xi,j) && (10)\\
&= \sum_{i=1}^{\xi-1} f(i,\xi) + \sum_{i=\xi+1}^{N} f(i,\xi) && (11)\\
&= \sum_{i=1}^{N} \left(1 - \delta_{i\xi}\right) f(i,\xi), && (12)
\end{aligned}
$$

where we have used that $f(i,j) = -f(j,i)$ (see Eq. 9). All in all:

$$
\textcircled{1} = \sum_{i=1}^{N} \left(1 - \delta_{i\xi}\right) \frac{4}{U_{i\xi}^2} \left(\vec{r}_\xi - \vec{r}_i\right) \max\left(0, \frac{\left(\vec{r}_\xi - \vec{r}_i\right)^2}{U_{i\xi}^2} - 1\right) \tag{13}
$$

Let us continue with $\textcircled{2}$. The chain rule gives:

$$
\frac{\partial}{\partial \vec{r}_\xi} \sum_{i<j}^{N} \max^2\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right) = 2\sum_{i<j}^{N} \max\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right) \frac{\partial}{\partial \vec{r}_\xi} \max\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right) \tag{14}
$$

For $\xi = i$,

$$
\frac{\partial}{\partial \vec{r}_i} \left(\frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right) = \frac{4L_{ij}^2 \left(\vec{r}_j - \vec{r}_i\right)}{\left(L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2\right)^2}, \tag{15}
$$

and likewise, but negative, for $\xi = j$. Therefore,

$$
\begin{aligned}
\frac{\partial}{\partial \vec{r}_\xi} \left(\max\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right)\right) &= \frac{4L_{ij}^2 \left(\vec{r}_j - \vec{r}_i\right)}{\left(L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2\right)^2} \left\{ \begin{array}{r|c} 1 & \xi = i \\ -1 & \xi = j \\ 0 & \text{else} \end{array} \right\} \\
&= \frac{4L_{ij}^2 \left(\vec{r}_j - \vec{r}_i\right)}{\left(L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2\right)^2} \left(\delta_{\xi i} - \delta_{\xi j}\right),
\end{aligned}
$$

where we have excluded the possibility of $\frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1 < 0$ since this case is covered by the first maximum function. Altogether:

$$
\textcircled{2} = \sum_{i<j}^{N} \left(\delta_{\xi i} - \delta_{\xi j}\right) \underbrace{\frac{8L_{ij}^2 \left(\vec{r}_j - \vec{r}_i\right)}{\left(L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2\right)^2} \max\left(0, \frac{2L_{ij}^2}{L_{ij}^2 + \left(\vec{r}_j - \vec{r}_i\right)^2} - 1\right)}_{g(i,j)}. \tag{16}
$$

Transforming the summation:

$$
\begin{aligned}
\sum_{i<j}^{N} \left(\delta_{\xi i} - \delta_{\xi j}\right) g(i,j) &= -\sum_{i=1}^{\xi-1} g(i,\xi) + \sum_{j=\xi+1}^{N} g(\xi,j) && (17)\\
&= \sum_{i=1}^{\xi-1} g(\xi,i) + \sum_{i=\xi+1}^{N} g(\xi,i) && (18)\\
&= \sum_{i=1}^{N} \left(1 - \delta_{i\xi}\right) g(\xi,i), && (19)
\end{aligned}
$$

Where we have used $g(i,j) = -g(j,i)$ (see Eq. 16). All in all:

$$
\textcircled{2} = \sum_{i=1}^{N} \left(1 - \delta_{i\xi}\right) \frac{8L_{\xi i}^2 \left(\vec{r}_i - \vec{r}_\xi\right)}{\left(L_{\xi i}^2 + \left(\vec{r}_i - \vec{r}_\xi\right)^2\right)^2} \max\left(0, \frac{2L_{\xi i}^2}{L_{\xi i}^2 + \left(\vec{r}_i - \vec{r}_\xi\right)^2} - 1\right) \tag{20}
$$

2.2 Chiral error terms

Next, we consider 3 . Applying the chain rule gives:

$$\frac{\partial}{\partial \vec{r}_\xi} \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} \max^2 \left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right)$$

$$= 2 \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} \max \left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right) \frac{\partial}{\partial \vec{r}_\xi} \max \left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right)$$

The partial derivatives of $V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right)$ with respect to $\vec{r}_\xi$ are split into five cases. The index ξ can be an element of one of the four sets $S_\alpha, S_\beta, S_\gamma, S_\delta$ (and only one, since they are mutually disjoint) or not. The derivative for the last case is zero. In the remaining cases, one average vector $\vec{s}$ is a function of $\vec{r}_\xi$ but the rest are not. The partial derivative of any average vector $\vec{s}$ is:

$$\frac{\partial}{\partial \vec{r}_\xi} \vec{s}_\alpha = \frac{\partial}{\partial \vec{r}_\xi} \frac{1}{|S_\alpha|} \sum_{i=1}^{|S_\alpha|} \vec{r}_{S_{\alpha,i}} = \left\{ \begin{array}{r|r} \frac{1}{|S_\alpha|}\mathbf{I}_3 & \xi \in S_\alpha \\ 0 & \text{else} \end{array} \right\} \tag{21}$$

where $\mathbf{I}_3$ denotes the three dimensional identity matrix. The individual set membership cases are thus as follows:

$$S_\alpha \quad \frac{\partial}{\partial \vec{r}_\xi} \left\{ \left(\vec{s}_\alpha - \vec{s}_\delta\right)^T \cdot \left[\left(\vec{s}_\beta - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right)\right] \right\} \tag{22}$$

$$= \frac{\partial}{\partial \vec{r}_\xi} \left\{ \vec{s}_\alpha^T \cdot \left[\left(\vec{s}_\beta - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right)\right] \right\} - \vec{0} \tag{23}$$

$$= \frac{1}{|S_\alpha|} \left[\left(\vec{s}_\beta - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right)\right] \tag{24}$$

In shorthand notation, in which all $\vec{s}$ symbols are replaced by their subscripts:

$$S_\beta \quad \frac{\partial}{\partial \vec{r}_\xi} \left(\vec{\alpha} - \vec{\delta}\right)^T \cdot \left[\left(\vec{\beta} - \vec{\delta}\right) \times \left(\vec{\gamma} - \vec{\delta}\right)\right] \tag{25}$$

$$= \frac{\partial}{\partial \vec{r}_\xi} \left(\vec{\alpha} - \vec{\delta}\right)^T \cdot \left[\vec{\beta} \times \vec{\gamma} - \vec{\beta} \times \vec{\delta} - \vec{\delta} \times \vec{\gamma} + \underbrace{\vec{\delta} \times \vec{\delta}}_{=0} \right] \tag{26}$$

$$= \frac{\partial}{\partial \vec{r}_\xi} \left\{ \vec{\beta}^T \cdot \left[\vec{\gamma} \times \left(\vec{\alpha} - \vec{\delta}\right)\right] - \vec{\beta}^T \cdot \left[\vec{\delta} \times \left(\vec{\alpha} - \vec{\delta}\right)\right] \right\} - \vec{0} \tag{27}$$

$$= \frac{1}{|S_\beta|} \left(\vec{\gamma} - \vec{\delta}\right) \times \left(\vec{\alpha} - \vec{\delta}\right) = -\frac{1}{|S_\beta|} \left(\vec{\alpha} - \vec{\delta}\right) \times \left(\vec{\gamma} - \vec{\delta}\right) \tag{28}$$

$$S_\gamma \quad \frac{\partial}{\partial \vec{r}_\xi} \left(\vec{\alpha} - \vec{\delta}\right)^T \cdot \left[\vec{\beta} \times \vec{\gamma} - \vec{\beta} \times \vec{\delta} - \vec{\delta} \times \vec{\gamma}\right] \tag{29}$$

$$= \frac{\partial}{\partial \vec{r}_\xi} \left\{ \vec{\gamma}^T \cdot \left[\left(\vec{\alpha} - \vec{\delta}\right) \times \vec{\beta}\right] - \vec{\gamma}^T \cdot \left[\left(\vec{\alpha} - \vec{\delta}\right) \times \vec{\delta}\right] \right\} - \vec{0} \tag{30}$$

$$= \left(\vec{\alpha} - \vec{\delta}\right) \times \left(\vec{\beta} - \vec{\delta}\right) \tag{31}$$

$$\textcircled{S_\delta} \quad \frac{\partial}{\partial \vec{r}_\xi} \left(\vec{\alpha} - \vec{\delta}\right)^T \cdot \left[\vec{\beta} \times \vec{\gamma} - \vec{\beta} \times \vec{\delta} - \vec{\delta} \times \vec{\gamma}\right] \tag{32}$$

$$= \frac{\partial}{\partial \vec{r}_\xi} \vec{\alpha}^T \cdot \left[\vec{\beta} \times \vec{\gamma} - \vec{\beta} \times \vec{\delta} - \vec{\delta} \times \vec{\gamma}\right] - \frac{\partial}{\partial \vec{r}_\xi} \vec{\delta}^T \cdot \left[\vec{\beta} \times \vec{\gamma} - \vec{\beta} \times \vec{\delta} - \vec{\delta} \times \vec{\gamma}\right] \tag{33}$$

$$= \underbrace{\frac{\partial}{\partial \vec{r}_\xi} \vec{\alpha}^T \cdot \left(\vec{\beta} \times \vec{\gamma}\right)}_{=0} - \frac{\partial}{\partial \vec{r}_\xi} \vec{\alpha}^T \cdot \left(\vec{\beta} \times \vec{\delta}\right) - \frac{\partial}{\partial \vec{r}_\xi} \vec{\alpha}^T \cdot \left(\vec{\delta} \times \vec{\gamma}\right) - \frac{\partial}{\partial \vec{r}_\xi} \vec{\delta}^T \cdot \left(\vec{\beta} \times \vec{\gamma}\right) + \frac{\partial}{\partial \vec{r}_\xi} \underbrace{\vec{\delta}^T \cdot \left(\vec{\delta} \times \vec{\gamma}\right)}_{=0} + \frac{\partial}{\partial \vec{r}_\xi} \underbrace{\vec{\delta}^T \cdot \left(\vec{\beta} \times \vec{\delta}\right)}_{=0} \tag{34}$$

$$= -\frac{\partial}{\partial \vec{r}_\xi} \vec{\delta}^T \cdot \left(\vec{\gamma} \times \vec{\alpha}\right) - \frac{\partial}{\partial \vec{r}_\xi} \vec{\delta}^T \cdot \left(\vec{\alpha} \times \vec{\beta}\right) - \frac{\partial}{\partial \vec{r}_\xi} \vec{\delta}^T \cdot \left(\vec{\beta} \times \vec{\gamma}\right) \tag{35}$$

$$= -\frac{1}{|S_\delta|} \vec{\gamma} \times \vec{\alpha} - \frac{1}{|S_\delta|} \vec{\alpha} \times \vec{\beta} - \frac{1}{|S_\delta|} \vec{\beta} \times \vec{\gamma} \tag{36}$$

$$= -\frac{1}{|S_\delta|} \left(\vec{\alpha} - \vec{\gamma}\right) \times \left(\vec{\beta} - \vec{\gamma}\right) \tag{37}$$

So, overall:

$$\textcircled{3} = \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} 2 \max\left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right) \left\{ \begin{array}{r|l} \frac{1}{|S_\alpha|} \left(\vec{s}_\beta - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right) & \xi \in S_\alpha \\ -\frac{1}{|S_\beta|} \left(\vec{s}_\alpha - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right) & \xi \in S_\beta \\ \frac{1}{|S_\gamma|} \left(\vec{s}_\alpha - \vec{s}_\delta\right) \times \left(\vec{s}_\beta - \vec{s}_\delta\right) & \xi \in S_\gamma \\ -\frac{1}{|S_\delta|} \left(\vec{s}_\alpha - \vec{s}_\gamma\right) \times \left(\vec{s}_\beta - \vec{s}_\gamma\right) & \xi \in S_\delta \\ 0 & \text{else} \end{array} \right\}. \tag{38}$$

For $\textcircled{4}$, the derivation is analog save for the sign of the great amount of cases, which we extrude from the sum:

$$\textcircled{4} = -\sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} 2 \max\left(0, L_V - V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right)\right) \left\{ \begin{array}{r|l} \frac{1}{|S_\alpha|} \left(\vec{s}_\beta - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right) & \xi \in S_\alpha \\ -\frac{1}{|S_\beta|} \left(\vec{s}_\alpha - \vec{s}_\delta\right) \times \left(\vec{s}_\gamma - \vec{s}_\delta\right) & \xi \in S_\beta \\ \frac{1}{|S_\gamma|} \left(\vec{s}_\alpha - \vec{s}_\delta\right) \times \left(\vec{s}_\beta - \vec{s}_\delta\right) & \xi \in S_\gamma \\ -\frac{1}{|S_\delta|} \left(\vec{s}_\alpha - \vec{s}_\gamma\right) \times \left(\vec{s}_\beta - \vec{s}_\gamma\right) & \xi \in S_\delta \\ 0 & \text{else} \end{array} \right\}. \tag{39}$$

Both terms concerning the chiral error can be summarized as follows:

$$\begin{aligned} \textcircled{3} + \textcircled{4} &= \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} 2 \max\left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right) \left\{\ldots\right\} \\ &- \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} 2 \max\left(0, L_V - V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right)\right) \left\{\ldots\right\} \\ &= \sum_{(S_\alpha, S_\beta, S_\gamma, S_\delta, U_V, L_V) \in C} 2 \left\{\ldots\right\} \left[\max\left(0, V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) - U_V\right) - \max\left(0, L_V - V_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right)\right)\right], \end{aligned}$$

which ought to save some time in an implementation.

2.3 Dihedral error terms

Finally, we consider 5. The chain rule yields:

$$\frac{\partial}{\partial \vec{r}_\xi} \sum_{(\dots)\in D} \max^2\left(0, h(\phi)\right) = 2 \sum_{(\dots)\in D} \max\left(0, h(\phi)\right) \frac{\partial}{\partial \vec{r}_\xi} \max\left(0, h(\phi)\right), \tag{40}$$

where we have abbreviated the dihedral expression in the maximum function with $h(\phi)$. We can drop the wrapping maximum function in the derivative since the first maximum function adequately covers the case $h(\phi) < 0$. Employing the chain rule yet again, we note $\frac{\partial}{\partial \vec{r}_\xi} h(\phi) = \frac{\partial h}{\partial \phi} \frac{\partial \phi}{\partial \vec{r}_\xi}$. The first part is:

$$\frac{\partial h}{\partial \phi} = \frac{\partial}{\partial \phi} \left| \underbrace{\phi_{\alpha\beta\gamma\delta}\left(\{\vec{r}_i\}\right) + \left\{ \begin{array}{c|l} 2\pi & \phi < \frac{U_\phi + L_\phi - 2\pi}{2} \\ 0 & \\ -2\pi & \phi > \frac{U_\phi + L_\phi + 2\pi}{2} \end{array} \right\} - \frac{U_\phi + L_\phi}{2}}_{w(\phi)} \right| - \frac{U_\phi - L_\phi}{2} = \operatorname{sgn}\left(w(\phi)\right). \tag{41}$$

The individual derivatives $\frac{\partial \phi}{\partial \vec{s}_\alpha}, \frac{\partial \phi}{\partial \vec{s}_\beta}, \frac{\partial \phi}{\partial \vec{s}_\gamma}, \frac{\partial \phi}{\partial \vec{s}_\delta}$ are given as:

$$\vec{f} = \left(\vec{s}_\alpha - \vec{s}_\beta\right), \quad \vec{g} = \left(\vec{s}_\beta - \vec{s}_\gamma\right), \quad \vec{h} = \left(\vec{s}_\delta - \vec{s}_\gamma\right), \quad \vec{a} = \vec{f} \times \vec{g}, \quad \vec{b} = \vec{h} \times \vec{g} \tag{42}$$

$$\begin{aligned} \frac{\partial \phi}{\partial \vec{s}_\alpha} &= -\frac{|\vec{g}|}{\vec{a}^{\,2}} \vec{a} \\ \frac{\partial \phi}{\partial \vec{s}_\beta} &= \frac{|\vec{g}|}{\vec{a}^{\,2}} \vec{a} + \frac{\vec{f}\vec{g}}{\vec{a}^{\,2}|\vec{g}|} \vec{a} - \frac{\vec{g}\vec{h}}{\vec{b}^{\,2}|\vec{g}|} \vec{b} \\ \frac{\partial \phi}{\partial \vec{s}_\gamma} &= -\frac{|\vec{g}|}{\vec{b}^{\,2}} \vec{b} + \frac{\vec{g}\vec{h}}{\vec{b}^{\,2}|\vec{g}|} \vec{b} - \frac{\vec{f}\vec{g}}{\vec{a}^{\,2}|\vec{g}|} \vec{a} \\ \frac{\partial \phi}{\partial \vec{s}_\delta} &= \frac{|\vec{g}|}{\vec{b}^{\,2}} \vec{b} \end{aligned} \tag{43}$$

The individual membership cases are thus:

$$S_i \qquad \frac{\partial \phi}{\partial \vec{r}_\xi} = \frac{\partial \phi}{\partial \vec{s}_i} \frac{\partial \vec{s}_i}{\partial \vec{r}_\xi} = \frac{1}{|S_i|} \frac{\partial \phi}{\partial \vec{s}_i} \tag{44}$$

And altogether:

$$5 = 2 \sum_{(\dots)\in D} \max(0, h(\phi)) \operatorname{sgn}(w(\phi)) \left\{ \begin{array}{r|c} \frac{1}{|S_\alpha|} \frac{\partial \phi}{\partial \vec{s_\alpha}} & \xi \in S_\alpha \\ \frac{1}{|S_\beta|} \frac{\partial \phi}{\partial \vec{s_\beta}} & \xi \in S_\beta \\ \frac{1}{|S_\gamma|} \frac{\partial \phi}{\partial \vec{s_\gamma}} & \xi \in S_\gamma \\ \frac{1}{|S_\delta|} \frac{\partial \phi}{\partial \vec{s_\delta}} & \xi \in S_\delta \\ 0 & \text{else} \end{array} \right\} \tag{45}$$