

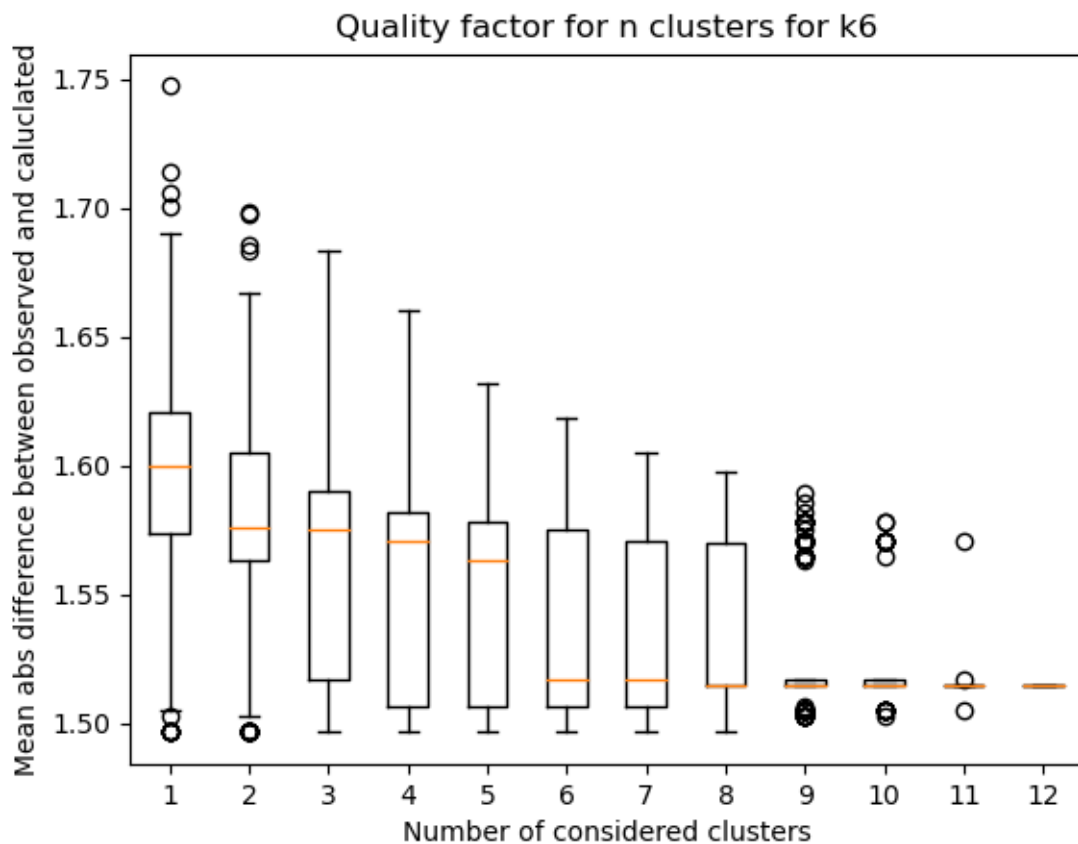
1 Summary for sPRE calculations with XPLORE

The summary of this project comprises three main points: Results, Problems, Methods

1.1 Results

Running XPLORE on MD data Th

How many clusters are needed? This question can be answered via this graph:



On the x-axis is the number of considered clusters. This includes all permutations, the 2 considered clusters are found by permuting over the

number of clusters: (0, 1), (0, 2), ... (0, 12), (1, 1), ... (1, 2), ... The y-axis is the mean abs difference between the calucaltion and the linear combination of the clusters. The linear combination was built as such:

$$\mathbf{sPRE} = v_m = x1 \cdot v_{c1} + x2 \cdot v_{c2} \dots \quad (1)$$

$$\mathbf{sPRE} = y = \begin{bmatrix} v(m, a) \\ \vdots \\ x_m \end{bmatrix} (sPRE_1, sPRE_2, \dots) = x1 * (sPRE_1, sPRE_2, sPRE_3), x2 * (sPRE_1, sPRE_2, sPRE_3) \dots \quad (2)$$