A screenshot of a cell phone

Description automatically generated

The minimum number of principal components I would use to represent the spectra would be 6, as it can be seen that it’s the ‘knee’ and after the 6th value they each begin to contribute less and less. If you needed high accuracy 39 could be used as that explains 99.95% of the variance. I will likely use a middle ground.

A close up of a map

Description automatically generated

This here shows the projection of the spectra on the 8 most important eigenvectors, and then scattering each combination of pairs. It can be seen that the graph in location [0, 1] would provide a good idea of separation. This indicates that the 1st and 2nd principal components may give the best separation