Plans for release II:

Bayesian PCA for improved noise robustness

Mixture of Bayesian PCA:s for modeling the nonlinear manifold that the in-plane aligned single-particle projections represents and improve classification for heterogeneity analysis. Use as generative model. Use for noise reduction and generation of representatives for alignment.

Bayesian model selection for ‘determining’ the number of states in a population.

Soft refinement. Perhaps it is idea to introduce the concept of a neighborhood in the weighting in the refinement. Have the DE sample the configuration space continuously and eject out solutions into a discrete structure of projection directions so that the in-plane degrees of freedom are kept ‘hard’ whereas the continuous projection directions are weighted according to a discrete projection direction structure with a neighborhood ‘enforcement’ (Path re-linking). Select a set of solutions that cluster in a region according to the resolution limit and weight within this region.

B factor scaling according to the highest profile in the data set.

Defocus parameter refinement.

Program for validate that takes as an input several ab initio reconstructions, docks them and measures the consistency between them somehow and assigns a resolution measure.