

aiPCAClassification

aiPCAClassification classifies a set of particles using the PCA method.

aiPCAClassification needs a configuration file provided by the **-u** argument. Some options can be overwritten using command line arguments.

Options are:

CudaDeviceIDs

The deviceIDs of the GPUs to use.

Argument for command line: **-d** or **--CudaDeviceIDs**

Type: **List<int>**, a list of integer values

Option is mandatory: **true**

LP

Low pass filter value.

Argument for command line: **-lp** or **--LP**

Type: **float**

Option is mandatory: **true**

LPS

Low pass filter sigma value.

Argument for command line: **-lps** or **--LPS**

Type: **float**

Option is mandatory: **true**

HP

High pass filter value.

Argument for command line: **-hp** or **--HP**

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**

HPS

High pass filter sigma value.

Argument for command line: **-hps** or **--HPS**

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**

StartWith

For a large number of particle, PCA classification can be a long process. To facilitate usage, the process can be split into multiple steps. This indicates the step to start processing with.

Type: one of [**COVAR_MATRIX**, **EIGEN_IMAGES**, **EIGEN_VALUES**, **KMEANS**, **SUM_CLASSES**, **SUM_PARTICLES**, **WEIGHT_MATRIX**]

Option is mandatory: **true**

Possible notations:

- **COVAR_MATRIX**: COVARMATRIX, COVAR-MATRIX, Covar-Matrix, covar-matrix, CovarMatrix, covarmatrix, COVAR_MATRIX

- **EIGEN_IMAGES:** EIGENIMAGES, EIGEN-IMAGES, Eigen-Images, eigen-images, EigenImages, eigenimages, EIGEN_IMAGES
- **EIGEN_VALUES:** EIGENVALUES, EIGEN-VALUES, Eigen-Values, eigen-values, EigenValues, eigenvalues, EIGEN_VALUES
- **KMEANS:** KMEANS, Kmeans, KMeans, kmeans
- **SUM_CLASSES:** SUMCLASSES, SUM-CLASSES, Sum-Classes, sum-classes, SumClasses, sum-classes, SUM_CLASSES
- **SUM_PARTICLES:** SUMPARTICLES, SUM-PARTICLES, Sum-Particles, sum-particles, SumParticles, sumparticles, SUM_PARTICLES
- **WEIGHT_MATRIX:** WEIGHTMATRIX, WEIGHT-MATRIX, Weight-Matrix, weight-matrix, WeightMatrix, weightmatrix, WEIGHT_MATRIX

EndWith

For a large number of particle, PCA classification can be a long process. To facilitate usage, the process can be split into multiple steps. This indicates the step to end processing with (inclusive).

Type: one of [**COVAR_MATRIX**, **EIGEN_IMAGES**, **EIGEN_VALUES**, **KMEANS**, **SUM_CLASSES**, **SUM_PARTICLES**, **WEIGHT_MATRIX**]

Option is mandatory: **true**

Possible notations:

- **COVAR_MATRIX:** COVARMATRIX, COVAR-MATRIX, Covar-Matrix, covar-matrix, CovarMatrix, covarmatrix, COVAR_MATRIX
- **EIGEN_IMAGES:** EIGENIMAGES, EIGEN-IMAGES, Eigen-Images, eigen-images, EigenImages, eigenimages, EIGEN_IMAGES
- **EIGEN_VALUES:** EIGENVALUES, EIGEN-VALUES, Eigen-Values, eigen-values, EigenValues, eigenvalues, EIGEN_VALUES
- **KMEANS:** KMEANS, Kmeans, KMeans, kmeans
- **SUM_CLASSES:** SUMCLASSES, SUM-CLASSES, Sum-Classes, sum-classes, SumClasses, sum-classes, SUM_CLASSES
- **SUM_PARTICLES:** SUMPARTICLES, SUM-PARTICLES, Sum-Particles, sum-particles, SumParticles, sumparticles, SUM_PARTICLES
- **WEIGHT_MATRIX:** WEIGHTMATRIX, WEIGHT-MATRIX, Weight-Matrix, weight-matrix, WeightMatrix, weightmatrix, WEIGHT_MATRIX

MotiveList

The list of particles to classify.

Type: **string**

Option is mandatory: **true**

MotiveListResult

The filename of the resulting motive list.

Type: **string**

Option is mandatory: **true**

Particles

Particle filename. Two naming conventions are possible: filename_PartNr.em/mrc or filename_TomoNr_PartInTomoNr.em/mr

Type: **string**

Option is mandatory: **true**

Wedges

Wedge filename. Naming convention: filename_WedgeNr.em/mrc.

Type: **string**

Option is mandatory: **true**

Mask

Mask filename.

Type: **string**

Option is mandatory: **true**

MaskFSC

Mask filename for the mask to use in FSC calculation.

Type: **string**

Option is mandatory: **true**

FourierFilterFileName

If set, the particles are not low and high pass filtered but filtered with the provided filter mask.

Type: **string**

Option is mandatory: **false**

Default value if not set: ""

NumberOfEigenvectors

The number of eigen vectors to compute.

Type: **int**

Option is mandatory: **true**

NumberOfClasses

The number of classes.

Type: **int**

Option is mandatory: **true**

NumberOfParticlesInPCA

Limit the number of particles used for the covariance matrix by randomly choosing X particles from the motivelist. Uses all particles if set to 0.

Type: **int**

Option is mandatory: **true**

BlockSize

To speed up calucations, the covariance matrix is computed in blocks of the given size.

Type: **int**

Option is mandatory: **true**

CovarMatrixFilename

The filename for the covariance matrix (.em format).

Type: **string**

Option is mandatory: **true**

WeightMatrixFilename

The filename for the weight matrix (.em format).

Type: **string**

Option is mandatory: **true**

EigenImagesFilename

The filename for the eigen images. Naming convention: filename__Nr.em/mrc.

Type: **string**

Option is mandatory: **true**

EigenVectorsFilename

The filename for the eigen vector (.em format).

Type: **string**

Option is mandatory: **false**

Default value if not set: **"**

EigenValuesFilename

The filename for the eigen values (.em format).

Type: **string**

Option is mandatory: **false**

Default value if not set: **"**

AverageParticleFile

The filename for the average of all particles (.em or .mrc format).

Type: **string**

Option is mandatory: **false**

Default value if not set: **"**

SumClassesFilename

The filename for the sum of each class. Naming convention: filename__ClassNr__IterationNr.em/mrc.

Type: **string**

Option is mandatory: **false**

Default value if not set: **"**

SumClassesIterationNumber

The iteration number to use in SumClassesFilename. Default: 0.

Type: **int**

Option is mandatory: **false**

Default value if not set: **0**