

Agglomerative Hierarchical Clustering

The C++ implementation for [AHC](#) with OpenMP

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Chapter 1

Agglomerative Hierarchical Clustering (AHC)

The program includes basically two aspects of [AHC](#)

- [AHC](#) of three linkages (will generate cluster result information)
 - Single linkage
 - Complete linkage
 - Average linkage
- The hierarchical L method to find optimal number of clusters (only generate optimal cluster number)
 - It is a global search of knee point along the clusters

Number of clusters as input

The program supports two kinds of input for number of clusters

- Direct input after the query information > Input cluster number among [0, 1000] for norm X:
- Read the cluster numbers from a txt file
 - The txt file is called 'cluster_number' in the /dataset/ folder
 - The 'cluster number' has the following format
0:10 // for similarity measure 0, the input of cluster number is 10 1:10 // for similarity measure 1, the input of cluster number is 10 2:10 4:10 12:10 13:10 14:10 15:10 17:10
for better batch processing especially in our experiment when the code is automatically run on the server

Chapter 2

Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

AHC	7
DataSet	22
DistNode	23
Ensemble	24

Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

AHC.cpp	27
AHC.h	27
main.cpp	27
Predefined.cpp	28
Predefined.h	28

Chapter 4

Class Documentation

4.1 AHC Class Reference

```
#include <AHC.h>
```

Collaboration diagram for AHC:

Public Member Functions

- [AHC](#) ()
- [AHC](#) (const int &argc, char **argv)
- [~AHC](#) ()
- void [performClustering](#) ()

Private Member Functions

- void [extractFeatures](#) (const std::vector< int > &storage, const std::vector< std::vector< int > > &neighborVec, const Eigen::MatrixXf ¢roid)
- void [setDataset](#) (const int &argc, char **argv)
- const float [getDistAtNodes](#) (const vector< int > &firstList, const vector< int > &secondList, const int &Linkage)
- void [hierarchicalMerging](#) (std::unordered_map< int, [Ensemble](#) > &node_map, std::vector< [DistNode](#) > &dNodeVec, std::vector< [Ensemble](#) > &nodeVec)
- void [setLabel](#) (const std::vector< [Ensemble](#) > &nodeVec, vector< vector< int > > &neighborVec, vector< int > &storage, Eigen::MatrixXf ¢roid)
- string [getLinkageStr](#) ()
- void [getEntropyRatio](#) (const std::vector< int > &storage, float &EntropyRatio)
- string [getNormStr](#) ()
- string [getEntropyStr](#) (const float &EntropyRatio)
- void [setValue_merge](#) (std::vector< [DistNode](#) > &dNodeVec, std::unordered_map< int, [Ensemble](#) > &node_map)
- void [setValue](#) (std::vector< [DistNode](#) > &dNodeVec, std::unordered_map< int, [Ensemble](#) > &node_map)
- void [performClustering_by_norm](#) ()

Private Attributes

- MetricPreparation [object](#)
- int [normOption](#)
- bool [isPBF](#)
- std::vector< int > [group](#)
- std::vector< string > [activityList](#)
- std::vector< string > [timeList](#)
- [DataSet](#) [ds](#)
- int [numberOfClusters](#)
- int [initializationOption](#)
- int [linkageOption](#)
- bool [lMethod](#)
- bool [readCluster](#)
- bool [isPathlines](#)
- std::vector< float > [curveValue](#) [4]

4.1.1 Detailed Description

Definition at line 36 of file AHC.h.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 AHC::AHC ()

Definition at line 12 of file AHC.cpp.

```
13 {  
14  
15 }
```

4.1.2.2 AHC::AHC (const int & *argc*, char ** *argv*)

Definition at line 26 of file AHC.cpp.

```
27 {  
28     setDataset(argc, argv);  
29 }
```

4.1.2.3 AHC::~AHC ()

Definition at line 38 of file AHC.cpp.

```
39 {  
40     deleteDistanceMatrix(ds.dataMatrix.rows\(\));  
41 }
```

4.1.3 Member Function Documentation

4.1.3.1 `void AHC::extractFeatures (const std::vector< int > & storage, const std::vector< std::vector< int > > & neighborVec, const Eigen::MatrixXf & centroid) [private]`

Definition at line 473 of file AHC.cpp.

```

475 {
476     const int& Row = ds.dataMatrix.rows();
477     const int& Column = ds.dataMatrix.cols();
478
479     std::cout << "Final group number information: " << std::endl;
480     for (int i = 0; i < storage.size(); ++i)
481     {
482         std::cout << storage[i] << " ";
483     }
484     std::cout << std::endl;
485
486     /* record labeling information */
487     // IOHandler::generateGroups(neighborVec);
488
489     IOHandler::printClusters(ds.dataVec, group, storage, "norm"+to_string(
normOption), ds.fullName, ds.dimension);
490
491     struct timeval start, end;
492     double timeTemp;
493
494     /* compute the centroid coordinates of each clustered group */
495
496     gettimeofday(&start, NULL);
497
498     vector<vector<float>> > closest(numberOfClusters);
499     vector<vector<float>> > furthest(numberOfClusters);
500
501     /* extract the closest and furthest streamlines to centroid */
502     #pragma omp parallel for schedule(static) num_threads(8)
503     for (int i=0; i<numberOfClusters; ++i)
504     {
505         float minDist = FLT_MAX;
506         float maxDist = -10;
507         int minIndex = -1, maxIndex = -1;
508         const std::vector<int>& groupRow = neighborVec[i];
509         const Eigen::VectorXf& eachCentroid = centroid.row(i);
510         for (int j = 0; j < groupRow.size(); ++j)
511         {
512             float distance = getDisimilarity(eachCentroid, ds.dataMatrix, groupRow[j],
normOption, object);
513             if(minDist>distance)
514             {
515                 minDist = distance;
516                 minIndex = groupRow[j];
517             }
518             if(maxDist<distance)
519             {
520                 maxDist = distance;
521                 maxIndex = groupRow[j];
522             }
523         }
524         closest[i] = ds.dataVec[minIndex];
525         furthest[i] = ds.dataVec[maxIndex];
526     }
527
528     /* re-assign centroid coordinates to the vector<vector<float>> */
529     std::vector<std::vector<float>> > center_vec(numberOfClusters, vector<float>(Column));
530     #pragma omp parallel for schedule(static) num_threads(8)
531     for (int i = 0; i < center_vec.size(); ++i)
532     {
533         for (int j = 0; j < Column; ++j)
534         {
535             center_vec[i][j] = centroid(i, j);
536         }
537     }
538
539     /* calculate the normalized entropy */
540     float EntropyRatio;
541     getEntropyRatio(storage, EntropyRatio);
542
543     std::cout << "Entropy ratio is: " << EntropyRatio << std::endl;
544
545     /* record the time for feature extraction */
546     gettimeofday(&end, NULL);

```

```

547     timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u
548                 + end.tv_usec - start.tv_usec) / 1.e6;
549     activityList.push_back("Feature extraction for norm "+to_string(
normOption)+ " takes: ");
550     timeList.push_back(to_string(timeTemp)+" s");
551
552     // calculate the normalized validity measurement
553     ValidityMeasurement vm;
554     vm.computeValue(normOption, ds.dataMatrix, group, object,
isPBF);
555     activityList.push_back("AHC Validity measure is: ");
556     stringstream fc_ss;
557     fc_ss << vm.f_c;
558     timeList.push_back(fc_ss.str());
559
560     // calculate the silhouette, the Gamma statistics and DB index
561     gettimeofday(&start, NULL);
562     Silhouette sil;
563     sil.computeValue(normOption, ds.dataMatrix, ds.
dataMatrix.rows(), ds.dataMatrix.cols(),
564                     group, object, numberOfClusters,
isPBF);
565     gettimeofday(&end, NULL);
566     timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u
567                 + end.tv_usec - start.tv_usec) / 1.e6;
568     activityList.push_back("Silhouette calculation for norm " +to_string(
normOption)+" takes: ");
569     timeList.push_back(to_string(timeTemp)+" s");
570
571     std::cout << "Finishing extracting features!" << std::endl;
572
573     stringstream ss;
574     ss << "norm_" << normOption;
575
576     /* measure closest and furthest rotation */
577     std::vector<float> closestRotation, furthestRotation;
578     const float& closestAverage = getRotation(closest, closestRotation);
579     const float& furthestAverage = getRotation(furthest, furthestRotation);
580
581     // record the linkage type, norm option and normalized entropy
582     string linkage = getLinkageStr();
583     string normStr = getNormStr();
584     string entropyStr = getEntropyStr(EntropyRatio);
585
586     // create the .vtk for streamline labels and cluster representatives
587     IOHandler::printFeature(ds.dataName+"_AHC_"+linkage+"_closest_"+ss.str()+".vtk", closest, sil
.sCluster,
588                             closestRotation, ds.dimension);
589     IOHandler::printFeature(ds.dataName+"_AHC_"+linkage+"_furthest_"+ss.str()+".vtk", furthest,
sil.sCluster,
590                             furthestRotation, ds.dimension);
591     IOHandler::printFeature(ds.dataName+"_AHC_"+linkage+"_centroid_"+ss.str()+".vtk", center_vec,
sil.sCluster, ds.dimension);
592
593     IOHandler::printToFull(ds.dataVec, sil.sData, "AHC_SValueLine_"+ss.str(),
ds.fullName, ds.dimension);
594     IOHandler::printToFull(ds.dataVec, group, sil.sCluster, "AHC_SValueCluster_"+ss.str(),
ds.fullName, ds.dimension);
595
596     // generate README for evaluation metrics
597     activityList.push_back("numCluster is: ");
598     timeList.push_back(to_string(numberOfClusters));
599
600     activityList.push_back("Average Silhouette is: ");
601     timeList.push_back(to_string(sil.sAverage));
602
603     activityList.push_back("Average rotation of closest is: ");
604     timeList.push_back(to_string(closestAverage));
605
606     activityList.push_back("Average rotation of furthest is: ");
607     timeList.push_back(to_string(furthestAverage));
608
609     IOHandler::generateReadme(activityList, timeList);
610     IOHandler::writeReadme("Linkage: "+linkage+" "+norm option is "+normStr+" ");
611     IOHandler::writeGroupSize(storage);
612
613     /* print entropy value for the clustering algorithm */
614     IOHandler::writeReadme(EntropyRatio, sil, "For norm "+to_string(normOption));
615     IOHandler::writeReadme(closestAverage, furthestAverage);
616
617     //curveValue[0].push_back(sil.sAverage);
618     //curveValue[1].push_back(sil.gammaStatistic);
619     //curveValue[2].push_back(sil.dbIndex);
620     //curveValue[3].push_back(vm.f_c);
621 }

```


4.1.3.2 const float AHC::getDistAtNodes (const vector< int > & firstList, const vector< int > & secondList, const int & Linkage) [private]

Definition at line 722 of file AHC.cpp.

```

723 {
724     const int& m = firstList.size();
725     const int& n = secondList.size();
726     assert(m!=0);
727     assert(n!=0);
728     /* 0: single linkage, min(x_i,y_j)
729      * 1: complete linkage, max(x_i,y_j)
730      * 2: average linkage, sum(x_i/y_j)
731      */
732     float result, value;
733     switch(Linkage)
734     {
735     case 0: //single linkage
736         {
737             result = FLT_MAX;
738             #pragma omp parallel for reduction(min:result) num_threads(8)
739             for(int i=0;i<m;++i)
740             {
741                 for(int j=0;j<n;++j)
742                 {
743                     if(distanceMatrix)
744                         value = distanceMatrix[firstList[i]][secondList[j]];
745                     else
746                         value = getDisimilarity(ds.dataMatrix, firstList[i], secondList[j],
normOption, object);
747                     result = std::min(result, value);
748                 }
749             }
750             break;
751         }
752     case 1: //complete linkage
753         {
754             result = -1.0;
755             #pragma omp parallel for reduction(max:result) num_threads(8)
756             for(int i=0;i<m;++i)
757             {
758                 for(int j=0;j<n;++j)
759                 {
760                     if(distanceMatrix)
761                         value = distanceMatrix[firstList[i]][secondList[j]];
762                     else
763                         value = getDisimilarity(ds.dataMatrix, firstList[i], secondList[j],
normOption, object);
764                     result = std::max(result, value);
765                 }
766             }
767             break;
768         }
769     case 2: // average linkage
770         {
771             result = 0;
772             #pragma omp parallel for reduction(+:result) num_threads(8)
773             for(int i=0;i<m;++i)
774             {
775                 for(int j=0;j<n;++j)
776                 {
777                     if(distanceMatrix)
778                         value = distanceMatrix[firstList[i]][secondList[j]];
779                     else
780                         value = getDisimilarity(ds.dataMatrix, firstList[i], secondList[j],
normOption, object);
781                     result+=value;
782                 }
783             }
784             result/=m*n;
785             break;
786         }
787     default: // no linkage option, should print "Error" information and exit the program
788         {
789             std::cout << "error!" << std::endl;
790             exit(1);
791         }
792     }
793     return result;
794 }
795 }
```

4.1.3.3 void AHC::getEntropyRatio (const std::vector< int > & storage, float & EntropyRatio) [private]

Definition at line 829 of file AHC.cpp.

```

830 {
831     EntropyRatio = 0;
832     const int& Row = ds.dataMatrix.rows();
833     for (int i = 0; i < storage.size(); ++i)
834     {
835         float ratio = float(storage[i])/float(Row);
836         EntropyRatio-=ratio*log2f(ratio);
837     }
838     EntropyRatio/=log2f(storage.size());
839 }
```

4.1.3.4 string AHC::getEntropyStr (const float & EntropyRatio) [private]

Definition at line 860 of file AHC.cpp.

```

861 {
862     stringstream ss;
863     ss << EntropyRatio;
864     return ss.str();
865 }
```

4.1.3.5 string AHC::getLinkageStr () [private]

Definition at line 802 of file AHC.cpp.

```

803 {
804     string result;
805     switch(linkageOption)
806     {
807     case 0:
808         result = "single";
809         break;
810     case 1:
811         result = "complete";
812         break;
813     case 2:
814         result = "average";
815         break;
816     }
817     return result;
818 }
```

4.1.3.6 string AHC::getNormStr () [private]

Definition at line 846 of file AHC.cpp.

```

847 {
848     stringstream ss;
849     ss << normOption;
850     return ss.str();
851 }
```

4.1.3.7 void AHC::hierarchicalMerging (std::unordered_map< int, Ensemble > & node_map, std::vector< DistNode > & dNodeVec, std::vector< Ensemble > & nodeVec) [private]

Definition at line 270 of file AHC.cpp.

```

272 {
273     std::map<int, float> dist_map;
274
275     /* would store distance matrix instead because it would save massive time */
276     struct timeval start, end;
277     double timeTemp;
278     gettimeofday(&start, NULL);
279
280     const int Row = ds.dataMatrix.rows();
281
282     DistNode popped;
283
284     /* find node-pair with minimal distance */
285     float minDist = FLT_MAX;
286     int target = -1;
287     for (int i = 0; i < dNodeVec.size(); ++i)
288     {
289         if(dNodeVec[i].distance<minDist)
290         {
291             target = i;
292             minDist = dNodeVec[i].distance;
293         }
294     }
295
296     // find which distNode is to be popped
297     popped = dNodeVec[target];
298
299     int index = Row, currentNumber;
300     do // perform iterative hierarchical merging until the final cluster reaches the given input number
301     {
302         if(lMethod) // if the l-method is enabled, record the number of clusters and merged
distance
303         {
304             dist_map.insert(std::make_pair(node_map.size(), popped.distance));
305         }
306         //create new node merged and input it into hash unordered_map
307         vector<int> first = (node_map[popped.first]).element;
308         vector<int> second = (node_map[popped.second]).element;
309
310         /* index would be starting from Row */
311         Ensemble newNode(index);
312         newNode.element = first;
313         newNode.element.insert(newNode.element.end(), second.begin(), second.end());
314         node_map.insert(make_pair(index, newNode));
315
316         //delete two original nodes
317         node_map.erase(popped.first);
318         node_map.erase(popped.second);
319
320         /* the difficulty lies how to update the min-heap with linkage
321          * This would take 2NlogN.
322          * Copy all node-pairs that are not relevant to merged nodes to new vec.
323          * For relevant, would update the mutual distance by linkage
324          */
325
326         /* how many clusters exist */
327         currentNumber = node_map.size();
328
329         target = -1, minDist = FLT_MAX;
330
331         // create new distNode vector
332         std::vector<DistNode> tempVec(currentNumber*(currentNumber-1)/2);
333
334         // update and find the minimal distance for next merging
335         int current = 0, i_first, i_second;
336         for(int i=0;i<dNodeVec.size();++i)
337         {
338             i_first=dNodeVec[i].first, i_second=dNodeVec[i].second;
339             /* not relevant, directly copied to new vec */
340             if(i_first!=popped.first&&i_first!=popped.second&&i_second!=popped.
first&&i_second!=popped.second)
341             {
342                 tempVec[current]=dNodeVec[i];
343                 if(tempVec[current].distance<minDist)
344                 {
345                     target = current;
346                     minDist = tempVec[current].distance;
347                 }

```

```

348         ++current;
349     }
350 }
351
352 // merge two nodes and update the node-distance relative to these two nodes
353 for (auto iter=node_map.begin(); iter!=node_map.end(); ++iter)
354 {
355     if ((*iter).first!=newNode.index)
356     {
357         tempVec[current].first = (*iter).first;
358         tempVec[current].second = newNode.index;
359         tempVec[current].distance=getDistAtNodes(newNode.element, (*iter).second.
element, linkageOption);
360         if(tempVec[current].distance<minDist)
361         {
362             target = current;
363             minDist = tempVec[current].distance;
364         }
365         ++current;
366     }
367 }
368
369 if(target>=0 && tempVec.size()>=1)
370 {
371     popped = tempVec[target];
372
373     /* judge whether current is assigned to right value */
374     assert(current==tempVec.size());
375     dNodeVec.clear();
376     dNodeVec = tempVec;
377     tempVec.clear();
378     ++index;
379 }
380
381 while(node_map.size() !=numberOfClusters); //merging happens whenever requested
cluster is not met
382
383 if(lMethod) // invoke the l-method to find the optimal number of clusters
384 {
385     /* perform L-method computation to detect optimal number of AHC */
386     DetermClusterNum dcn;
387     dcn.iterativeRefinement(dist_map);
388     std::cout << "Optimal number of clusters by L-Method is " << dcn.getFinalNumOfClusters() <<
std::endl;
389     dcn.recordLMethodResult(normOption);
390 }
391
392 else // otherwise, just perform the AHC clustering
393 {
394     nodeVec=std::vector<Ensemble>(node_map.size());
395     int tag = 0;
396     for(auto iter=node_map.begin(); iter!=node_map.end(); ++iter)
397         nodeVec[tag++]=(*iter).second;
398
399     gettimeofday(&end, NULL);
400     timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u + end.tv_usec - start.tv_usec) / 1.e6;
401
402     activityList.push_back("Hirarchical clustering of norm "+to_string(
normOption)+" for "+
403                             to_string(numberOfClusters)+" groups takes: ");
404     timeList.push_back(to_string(timeTemp)+" s");
405     /* task completed, would delete memory contents */
406     dNodeVec.clear();
407     node_map.clear();
408     /* use alpha function to sort the group by its size in ascending order */
409     std::sort(nodeVec.begin(), nodeVec.end(), [](const Ensemble& e1, const
Ensemble& e2)
410     {return e1.element.size()<e2.element.size() || (e1.element.size()==e2.element.size() &&
e1.index<e2.index);});
411 }
412 }

```

4.1.3.8 void AHC::performClustering ()

Definition at line 165 of file AHC.cpp.

```

166 {
167     /* 0: Euclidean Norm
168        1: Fraction Distance Metric
169        2: piece-wise angle average

```

```

170         3: Bhattacharyya metric for rotation
171         4: average rotation
172         5: signed-angle intersection
173         6: normal-direction multivariate distribution
174         7: Bhattacharyya metric with angle to a fixed direction
175         8: Piece-wise angle average \times standard deviation
176         9: normal-direction multivariate un-normalized distribution
177         10:  $x \cdot y / |x| \cdot |y|$  borrowed from machine learning
178         11: cosine similarity
179         12: Mean-of-closest point distance (MCP)
180         13: Hausdorff distance  $\min_{x_i, y_i}$ 
181         14: Signature-based measure from http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6231627
182         15: Procrustes distance take from http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6787131
183         16: entropy-based distance metric taken from http://vis.cs.ucdavis.edu/papers/pg2011paper.pdf
184         17: time-series MCP distance from https://www.sciencedirect.com/science/article/pii/S0097849318300128
185         for pathlines only
186     */
187
188     // read the input number for different similarity measures from the file "cluster_number"
189     std::unordered_map<int, int> clusterMap;
190     if(readCluster)
191     {
192         IOHandler::readClusteringNumber(clusterMap, "cluster_number");
193     }
194
195     // std::vector<int> cluster_array;
196     //for(int i=2; i<=100; ++i)
197     //{
198         //cluster_array.push_back(i);
199         for(normOption=0; normOption<=17; ++normOption)
200         {
201             if(isPathlines) // for pathlines, will consider d_T (17)
202             {
203                 if(normOption!=0 && normOption!=1 &&
204 normOption!=2 && normOption!=4 && normOption!=12
205                 && normOption!=13 && normOption!=14 &&
206 normOption!=15 && normOption!=17)
207                     continue;
208             }
209             else // for streamlines, will not consider d_T (17)
210             {
211                 if(normOption!=0 && normOption!=1 &&
212 normOption!=2 && normOption!=4 && normOption!=12
213                 && normOption!=13 && normOption!=14 &&
214 normOption!=15)
215                     continue;
216             }
217             std::cout << "-----" << std::endl;
218             std::cout << "norm " << normOption << " starts....." << std::endl;
219             timeList.clear();
220             activityList.clear();
221
222             /* L-method is not performed. It's a normal AHC procedure */
223             if(!lMethod)
224             {
225                 const int& Row = ds.dataMatrix.rows();
226                 if(readCluster)
227                 {
228                     numberOfClusters = clusterMap[normOption];
229                 }
230                 else
231                 {
232                     std::cout << "-----" << std::endl;
233                     std::cout << "Input cluster number among [0, " << Row << "]" for norm " <<
234 normOption << ": ";
235                     std::cin >> numberOfClusters;
236                     assert(numberOfClusters>0 && numberOfClusters<Row);
237                 }
238                 //numberOfClusters = i;
239                 assert(numberOfClusters>0 && numberOfClusters<Row);
240             }
241             /* perform L-method for detecting optimal num of clusters */
242             else if(lMethod)
243             {
244                 numberOfClusters = 1;
245             }
246             // perform clustering by given input of norm option
247             performClustering_by_norm();
248         }
249     }
250
251     //}
252
253     //std::ofstream curve("../dataset/curveValue.txt", ios::out);
254     for(int i=0; i<4; ++i)
255     {
256         for(int j=0; j<curveValue[0].size(); ++j)
257         {

```

```

251         curve << curveValue[i][j] << " ";
252     }
253     curve << std::endl;
254 }
255 curve.close();*/
256 }

```

4.1.3.9 void AHC::performClustering_by_norm() [private]

Definition at line 53 of file AHC.cpp.

```

54 {
55     /* very hard to decide whether needed to perform such pre-processing, but still create a
56      * MetricPreparation object in case some pre-calculation for similarity measures can be ready
57      * before the pairwise distance matrix calculation
58      */
59     object = MetricPreparation(ds.dataMatrix.rows(), ds.dataMatrix.cols());
60     object.preprocessing(ds.dataMatrix, ds.dataMatrix.rows(),
61         ds.dataMatrix.cols(), normOption);
62
63     /* would store distance matrix instead because it would save massive time */
64     struct timeval start, end;
65     double timeTemp;
66     gettimeofday(&start, NULL);
67
68     // check whether the file for distance matrix exists or not
69     std::ifstream distFile("../dataset/"+to_string(normOption)).c_str(), ios::in);
70     if(distFile.fail()) // not exist, will calculate the distance matrix and store them in local files
71     {
72         distFile.close();
73         // calculate the distance matrix
74         getDistanceMatrix(ds.dataMatrix, normOption, object);
75         // store the distance matrix values in the local files
76         std::ofstream distFileOut("../dataset/"+to_string(normOption)).c_str(), ios::out);
77         for(int i=0; i<ds.dataMatrix.rows(); ++i)
78         {
79             for(int j=0; j<ds.dataMatrix.rows(); ++j)
80             {
81                 distFileOut << distanceMatrix[i][j] << " ";
82             }
83             distFileOut << std::endl;
84         }
85         distFileOut.close();
86     }
87     else // the file for distance matrix exists, then directly reads in the pair-wise values
88     {
89         std::cout << "read distance matrix..." << std::endl;
90
91         distanceMatrix = new float*[ds.dataMatrix.rows()];
92         #pragma omp parallel for schedule(static) num_threads(8)
93         for (int i = 0; i < ds.dataMatrix.rows(); ++i)
94         {
95             distanceMatrix[i] = new float[ds.dataMatrix.rows()];
96         }
97
98         // read the distance values from the .txt file
99         int i=0, j;
100         string line;
101         stringstream ss;
102         while(getline(distFile, line))
103         {
104             j=0;
105             ss.str(line);
106             while(ss>>line)
107             {
108                 if(i==j)
109                     distanceMatrix[i][j]=0;
110                 else
111                     distanceMatrix[i][j] = std::atof(line.c_str());
112                 ++j;
113             }
114             ++i;
115             ss.str("");
116             ss.clear();
117         }
118         distFile.close();
119     }
120
121     // record the time for distance matrix computation time
122     gettimeofday(&end, NULL);

```

```

122     timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u
123               + end.tv_usec - start.tv_usec) / 1.e6;
124     activityList.push_back("Distance matrix computing for norm "+to_string(
normOption)+" takes: ");
125     timeList.push_back(to_string(timeTemp)+" s");
126
127     // create node-related parameters for AHC clustering
128     std::unordered_map<int, Ensemble> node_map;
129     std::vector<DistNode> dNodeVec;
130     std::vector<Ensemble> nodeVec;
131
132     /* set the ditNode vector */
133     setValue_merge(dNodeVec, node_map);
134
135     /* perform hiarchical clustering where within each step would merge two nodes */
136     hierarchicalMerging(node_map, dNodeVec, nodeVec);
137
138     if(!lMethod) // perform the AHC clustering with lMethod not activated
139     {
140         vector<vector<int>> neighborVec(numberOfClusters);
141         // element size for all groups
142         vector<int> storage(numberOfClusters);
143
144         // geometric center
145         Eigen::MatrixXf centroid = Eigen::MatrixXf::Zero(numberOfClusters,
ds.dataMatrix.cols());
146
147         // set label information
148         setLabel(nodeVec, neighborVec, storage, centroid);
149
150         nodeVec.clear();
151
152         extractFeatures(storage, neighborVec, centroid);
153     }
154 }

```

4.1.3.10 void AHC::setDataset (const int & argc, char ** argv) [private]

Definition at line 634 of file AHC.cpp.

```

635 {
636     if(argc!=3)
637     {
638         std::cout << "Input argument should have 3!" << endl
639                 << ". /cluster inputFile_name(in dataset folder) "
640                 << "data_dimension(3)" << endl;
641         exit(1);
642     }
643     // get the attribute for data set
644     ds.strName = string("../dataset/") + string(argv[1]);
645     ds.dataName = string(argv[1]);
646     ds.dimension = atoi(argv[2]);
647
648     /* get the bool tag for isPBF */
649     std::cout << "It is a PBF dataset? 1.Yes, 0.No" << std::endl;
650     int PBFjudgement;
651     std::cin >> PBFjudgement;
652     assert(PBFjudgement==1||PBFjudgement==0);
653     isPBF = (PBFjudgement==1);
654
655     /* get the bool tag for isPBF */
656     std::cout << "It is a pathline dataset? 1.Yes, 0.No" << std::endl;
657     std::cin >> PBFjudgement;
658     assert(PBFjudgement==1||PBFjudgement==0);
659     isPathlines = (PBFjudgement==1);
660
661     // set up the sample option by user input and data set type (pathlines or streamlines)
662     int sampleOption;
663     if(isPathlines) // default direct-repeating for pathlines to match the time steps
664         sampleOption = 1;
665     else // streamline sample option can be versatile
666     {
667         std::cout << "choose a sampling method for the dataset?" << std::endl
668                 << "1.directly filling with last vertex; 2. uniform sampling." << std::endl;
669         std::cin >> sampleOption;
670         assert(sampleOption==1||sampleOption==2);
671     }
672
673     // read the coordinates into the member variables
674     IOHandler::readFile(ds.strName, ds.dataVec, ds.vertexCount,

```

```

        ds.dimension, ds.maxElements);
675
676 // get the path of full name and print the streamlines vtk
677 ds.fullName = ds.strName+"_full.vtk";
678 IOHandler::printVTK(ds.fullName, ds.dataVec, ds.
vertexCount, ds.dimension);
679
680 // perform sampling operation with user parameters
681 if(sampleOption==1)
682     IOHandler::expandArray(ds.dataMatrix, ds.dataVec, ds.
dimension, ds.maxElements);
683 else if(sampleOption==2)
684     IOHandler::sampleArray(ds.dataMatrix, ds.dataVec, ds.
dimension, ds.maxElements);
685
686 // create the label index for each individual streamline/pathline
687 group = std::vector<int>(ds.dataMatrix.rows());
688
689 // whether to activate the L-method or not
690 std::cout << "Perform L-method to detect optimal num of clusters? 0: No, 1: Yes! " << std::endl;
691 std::cin >> lMethod;
692 assert(lMethod==0 || lMethod==1);
693 lMethod = (lMethod==1);
694
695 // which linkage type to be selected
696 std::cout << "-----" << std::endl;
697 std::cout << "Input linkage option: 0.single linkage, 1.complete linkage, 2.average linkage" <<
std::endl;
698 std::cin >> linkageOption;
699 assert(linkageOption==0||linkageOption==1||linkageOption==2);
700
701 // lMethod is not activated, so will ask for number of cluster as input
702 if(!lMethod)
703 {
704     std::cout << "-----" << std::endl;
705     std::cout << "Choose cluster number input method: 0.user input, 1.read from file: " << std::endl;
706     int clusterInput;
707     std::cin >> clusterInput;
708     assert(clusterInput==0||clusterInput==1);
709     readCluster = (clusterInput==1);
710 }
711 }

```

4.1.3.11 void AHC::setLabel (const std::vector< Ensemble > & nodeVec, vector< vector< int > > & neighborVec, vector< int > & storage, Eigen::MatrixXf & centroid) [private]

Definition at line 426 of file AHC.cpp.

```

428 {
429 // group tag by increasing order
430 int groupID = 0;
431
432 // element list for each group
433 vector<int> eachContainment;
434
435 // find group id and neighboring vec
436 for(auto iter = nodeVec.begin(); iter!=nodeVec.end(); ++iter)
437 {
438     eachContainment = (*iter).element;
439     neighborVec[groupID] = eachContainment;
440     #pragma omp parallel num_threads(8)
441     {
442         #pragma omp for nowait
443         for(int i=0; i<eachContainment.size(); ++i)
444         {
445             // update the label index for each streamline candidates
446             group[eachContainment[i]] = groupID;
447             #pragma omp critical
448             // update the centroid coordinates of the cluster
449             centroid.row(groupID) += ds.dataMatrix.row(eachContainment[i]);
450         }
451     }
452     storage[groupID] = (*iter).element.size();
453     centroid.row(groupID)/=eachContainment.size();
454     ++groupID;
455     eachContainment.clear();
456 }
457 }

```


4.1.3.12 `void AHC::setValue (std::vector< DistNode > & dNodeVec, std::unordered_map< int, Ensemble > & node_map) [private]`

Definition at line 955 of file AHC.cpp.

```

956 {
957     const int& Row = ds.dataMatrix.rows();
958     dNodeVec = std::vector<DistNode>(Row*(Row-1)/2);
959     int tag = 0;
960     // record the node i, node j and their distance into the vector
961     for(int i=0;i<Row-1;++i)
962     {
963         for(int j=i+1;j<Row;++j)
964         {
965             dNodeVec[tag].first = i;
966             dNodeVec[tag].second = j;
967             if(distanceMatrix)
968                 dNodeVec[tag].distance = distanceMatrix[i][j];
969             else
970                 dNodeVec[tag].distance = getDisimilarity(ds.dataMatrix, i, j,
normOption, object);
971             ++tag;
972         }
973     }
974     assert(tag==dNodeVec.size());
975     // record the index of the node
976     for(int i=0;i<Row;++i)
977     {
978         node_map[i].element.push_back(i);
979     }
980 }
```

4.1.3.13 `void AHC::setValue_merge (std::vector< DistNode > & dNodeVec, std::unordered_map< int, Ensemble > & node_map) [private]`

Definition at line 874 of file AHC.cpp.

```

875 {
876     const int& Row = ds.dataMatrix.rows();
877
878     /* find the node of closest distance */
879     std::vector<int> miniNode(Row);
880     #pragma omp parallel for schedule(static) num_threads(8)
881     for(int i=0;i<Row;++i)
882     {
883         float miniDist = FLT_MAX, dist;
884         int index = -1;
885         for(int j=0;j<Row;++j)
886         {
887             if(i==j)
888                 continue;
889             if(distanceMatrix)
890                 dist = distanceMatrix[i][j];
891             else
892                 dist = getDisimilarity(ds.dataMatrix, i, j,
normOption, object);
893
894             if(miniDist>dist)
895             {
896                 miniDist=dist;
897                 index=j;
898             }
899         }
900         miniNode[i]=index;
901     }
902
903     std::vector<bool> isIn(Row, false);
904
905     // update the map for node
906     int tag = 0;
907     for(int i=0;i<Row;++i)
908     {
909         if(!isIn[i])
910         {
911             Ensemble en;
```

```

912         if(miniNode[miniNode[i]]==i)
913         {
914             en.element.push_back(i);
915             en.element.push_back(miniNode[i]);
916             isIn[i]=true;
917             isIn[miniNode[i]]=true;
918             node_map[tag] = en;
919         }
920         else
921         {
922             en.element.push_back(i);
923             isIn[i]=true;
924             node_map[tag] = en;
925         }
926         ++tag;
927     }
928 }
929
930 // update the dNodeVec from the newly create nodes
931 const int& mapSize = node_map.size();
932 dNodeVec = std::vector<DistNode>(mapSize*(mapSize-1)/2);
933
934 tag = 0;
935 for(auto start = node_map.begin(); start!=node_map.end(); ++start)
936 {
937     for(auto end = node_map.begin(); end!=node_map.end() && end!=start; ++end)
938     {
939         dNodeVec[tag].first = start->first;
940         dNodeVec[tag].second = end->first;
941         dNodeVec[tag].distance = getDistAtNodes(start->second.element,end->second.element
942 , linkageOption);
943         ++tag;
944     }
945     assert(tag==dNodeVec.size());
946 }

```

4.1.4 Member Data Documentation

4.1.4.1 `std::vector<string> AHC::activityList` [private]

Definition at line 122 of file AHC.h.

4.1.4.2 `std::vector<float> AHC::curveValue[4]` [private]

Definition at line 167 of file AHC.h.

4.1.4.3 `DataSet AHC::ds` [private]

Definition at line 132 of file AHC.h.

4.1.4.4 `std::vector<int> AHC::group` [private]

Definition at line 117 of file AHC.h.

4.1.4.5 `int AHC::initializationOption` [private]

Definition at line 142 of file AHC.h.

4.1.4.6 `bool AHC::isPathlines` [private]

Definition at line 162 of file AHC.h.

4.1.4.7 `bool AHC::isPBF` [private]

Definition at line 112 of file AHC.h.

4.1.4.8 `int AHC::linkageOption` [private]

Definition at line 147 of file AHC.h.

4.1.4.9 `bool AHC::IMethod` [private]

Definition at line 152 of file AHC.h.

4.1.4.10 `int AHC::normOption` [private]

Definition at line 107 of file AHC.h.

4.1.4.11 `int AHC::numberOfClusters` [private]

Definition at line 137 of file AHC.h.

4.1.4.12 `MetricPreparation AHC::object` [private]

Definition at line 102 of file AHC.h.

4.1.4.13 `bool AHC::readCluster` [private]

Definition at line 157 of file AHC.h.

4.1.4.14 `std::vector<string> AHC::timeList` [private]

Definition at line 127 of file AHC.h.

The documentation for this class was generated from the following files:

- [AHC.h](#)
- [AHC.cpp](#)

4.2 DataSet Struct Reference

```
#include <Predefined.h>
```

Public Attributes

- `vector< vector< float > >` [dataVec](#)
- `Eigen::MatrixXf` [dataMatrix](#)
- `int` [maxElements](#) = -1
- `int` [vertexCount](#) = -1
- `int` [dimension](#) = -1
- `string` [strName](#)
- `string` [fullName](#)
- `string` [dataName](#)

4.2.1 Detailed Description

Definition at line 20 of file `Predefined.h`.

4.2.2 Member Data Documentation

4.2.2.1 `Eigen::MatrixXf DataSet::dataMatrix`

Definition at line 23 of file `Predefined.h`.

4.2.2.2 `string DataSet::dataName`

Definition at line 30 of file `Predefined.h`.

4.2.2.3 `vector<vector<float> > DataSet::dataVec`

Definition at line 22 of file `Predefined.h`.

4.2.2.4 `int DataSet::dimension = -1`

Definition at line 26 of file `Predefined.h`.

4.2.2.5 `string DataSet::fullName`

Definition at line 29 of file `Predefined.h`.

4.2.2.6 int DataSet::maxElements = -1

Definition at line 24 of file Predefined.h.

4.2.2.7 string DataSet::strName

Definition at line 28 of file Predefined.h.

4.2.2.8 int DataSet::vertexCount = -1

Definition at line 25 of file Predefined.h.

The documentation for this struct was generated from the following file:

- [Predefined.h](#)

4.3 DistNode Struct Reference

```
#include <Predefined.h>
```

Public Member Functions

- [DistNode](#) (const int &[first](#), const int &[second](#), const float &dist)
- [DistNode](#) ()

Public Attributes

- int [first](#) = -1
- int [second](#) = -1
- float [distance](#) = -1.0

4.3.1 Detailed Description

Definition at line 69 of file Predefined.h.

4.3.2 Constructor & Destructor Documentation

4.3.2.1 DistNode::DistNode (const int & *first*, const int & *second*, const float & *dist*) [inline]

Definition at line 74 of file Predefined.h.

```
74                                     :first(  
    first), second(second), distance(dist)  
75     {}
```

4.3.2.2 DistNode::DistNode () [inline]

Definition at line 77 of file Predefined.h.

```
78     {}
```

4.3.3 Member Data Documentation

4.3.3.1 float DistNode::distance = -1.0

Definition at line 72 of file Predefined.h.

4.3.3.2 int DistNode::first = -1

Definition at line 71 of file Predefined.h.

4.3.3.3 int DistNode::second = -1

Definition at line 71 of file Predefined.h.

The documentation for this struct was generated from the following file:

- [Predefined.h](#)

4.4 Ensemble Struct Reference

```
#include <Predefined.h>
```

Public Member Functions

- [Ensemble](#) (const int &[index](#))
- [Ensemble](#) ()

Public Attributes

- int [index](#) = -1
- std::vector< int > [element](#)

4.4.1 Detailed Description

Definition at line 38 of file Predefined.h.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 Ensemble::Ensemble (const int & *index*) [inline]

Definition at line 45 of file Predefined.h.

```
45                                     : index\(index\)  
46     {}
```

4.4.2.2 Ensemble::Ensemble () [inline]

Definition at line 48 of file Predefined.h.

```
49     {}
```

4.4.3 Member Data Documentation

4.4.3.1 std::vector<int> Ensemble::element

Definition at line 43 of file Predefined.h.

4.4.3.2 int Ensemble::index = -1

Definition at line 40 of file Predefined.h.

The documentation for this struct was generated from the following file:

- [Predefined.h](#)

Chapter 5

File Documentation

5.1 AHC.cpp File Reference

```
#include "AHC.h"
```

Include dependency graph for AHC.cpp:

5.2 AHC.h File Reference

```
#include <unordered_set>
#include <unordered_map>
#include <map>
#include <string>
#include <algorithm>
#include "Predefined.h"
#include "ValidityMeasurement.h"
#include "DetermClusterNum.h"
```

Include dependency graph for AHC.h: This graph shows which files directly or indirectly include this file:

Classes

- class [AHC](#)

5.3 main.cpp File Reference

```
#include "AHC.h"
```

Include dependency graph for main.cpp:

Functions

- int [main](#) (int argc, char **argv)

5.3.1 Function Documentation

5.3.1.1 `int main (int argc, char ** argv)`

Definition at line 17 of file main.cpp.

```
18 {
19     AHC ahc(argc, argv);
20     ahc.performClustering();
21     return 0;
22 }
```

5.4 Predefined.cpp File Reference

```
#include "Predefined.h"
```

Include dependency graph for Predefined.cpp:

Functions

- `template<class T >`
void `deleteVecElements` (`std::vector< T > &original`, `const T &first`, `const T &second`)

5.4.1 Function Documentation

5.4.1.1 `template<class T > void deleteVecElements (std::vector< T > & original, const T & first, const T & second)`

Definition at line 19 of file Predefined.cpp.

```
20 {
21     std::size_t size = original.size();
22     assert(size>2);
23     vector<T> result(size-2);
24     int tag = 0;
25     for(int i=0;i<size;++i)
26     {
27         //meet with target elements, not copied
28         if(original[i]==first || original[i]==second)
29             continue;
30         result[tag++]=original[i];
31     }
32     assert(tag==size-2);
33     original = result;
34 }
```

5.5 Predefined.h File Reference

```
#include "IOHandler.h"
#include "Initialization.h"
#include "Silhouette.h"
```

Include dependency graph for Predefined.h: This graph shows which files directly or indirectly include this file:

Classes

- struct [DataSet](#)
- struct [Ensemble](#)
- struct [DistNode](#)

Functions

- template<class T >
void [deleteVecElements](#) (std::vector< T > &origine, const T &first, const T &second)

5.5.1 Function Documentation

5.5.1.1 template<class T > void deleteVecElements (std::vector< T > & *origine*, const T & *first*, const T & *second*)

Definition at line 19 of file Predefined.cpp.

```
20 {  
21     std::size_t size = original.size();  
22     assert(size>2);  
23     vector<T> result (size-2);  
24     int tag = 0;  
25     for(int i=0;i<size;++i)  
26     {  
27         //meet with target elements, not copied  
28         if(original[i]==first || original[i]==second)  
29             continue;  
30         result[tag++]=original[i];  
31     }  
32     assert(tag==size-2);  
33     original = result;  
34 }
```

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