Affinity Propagation

The C++ implmentation for Affinity Propagation

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Chapter 1

Decription of Affinity Propagation

The implementation is an $O(n^3)$ with OpenMP and we have tested the result on the point cloud data set and compre it to the Frey Lab webpage linux binary version.

Two critical parameters are to be set

- Preference value s(i,i)
 - The preference value in affinity propagation and Frey Lab webpage is set to be the median of negative squared Euclidean distance between points
 - However, in flow visualization, it is set to be the minimal similarity value among streamlines
- · Relaxation factor lambda
 - It controls the update rate and the default value is 0.5
- · Max iteration
 - Due to that distance matrix for the streamline data sets is often large size (>3000*3000), the default value is 20

A two-level affinity propagation

Besides the conventional affinity propagation, the two-level affinity propagation is also included for user selection.

Chapter 2

Class Index

2.1 Class List

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

AffinityPropagation				 			 				 										
DataSet				 			 				 					 					2
Ensemble				 			 				 					 					2
Para																					2

4 Class Index

Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

AffinityPropagation.cpp	25
AffinityPropagation.h	25
main.cpp	26
Predefined.h	26

6 File Index

Chapter 4

Class Documentation

4.1 AffinityPropagation Class Reference

#include <AffinityPropagation.h>

Collaboration diagram for AffinityPropagation:

Public Member Functions

- AffinityPropagation ()
- AffinityPropagation (const int &argc, char **argv, const Para &p, bool &automatic)
- ∼AffinityPropagation ()
- void performClustering ()

Private Member Functions

- void extractFeatures (const std::vector< int > &storage, const std::vector< std::vector< int > > &neighbor
 — Vec, const Eigen::MatrixXf ¢roid)
- void setDataset (const int &argc, char **argv)
- void getParameterUserInput ()
- void setParameterAutomatic (const Para &p)
- void clusterByNorm (const int &norm)
- void setLabel (vector< vector< int > > &neighborVec, vector< int > &storage, Eigen::MatrixXf ¢roid, std::vector< int > &groupTag)
- void getEntropyRatio (const std::vector< int > &storage, float &EntropyRatio)
- void performAPClustering (Eigen::MatrixXf &matrixS, Eigen::MatrixXf &matrixA, Eigen::MatrixXf &matrixAf &matrixAf
- void getMatrixS (Eigen::MatrixXf &matrixS, float **distMatrix, const Eigen::MatrixXf &coordinates)
- void initializeMatrices (Eigen::MatrixXf &matrixS, Eigen::MatrixXf &matrixA, const int &rows)
- void updateResponsibility (Eigen::MatrixXf &matrixR, const Eigen::MatrixXf &matrixA, const Eigen::MatrixXf &matrixXf
 &matrixS)
- void updateAvailability (Eigen::MatrixXf &matrixA, const Eigen::MatrixXf &matrixR)
- void getGroupAssignment (const Eigen::MatrixXf &matrixR, const Eigen::MatrixXf &matrixXf &ma
- void getDistMatrixForCentroids (float ***centroidDistMatrix, const int &norm, const Eigen::MatrixXf ¢roid)
- void getDistanceMatrixFromFile (const int &norm)
- void getHierarchicalClusters (std::vector< int > &storage, std::vector< std::vector< int > > &neighbor←
 Vec, Eigen::MatrixXf ¢roid, std::vector< int > &group, const std::vector< int > ¢roidGroup, const int
 &groupSize)

Private Attributes

- MetricPreparation object
- int normOption = -1
- std::vector< int > group
- std::vector< string > activityList
- std::vector< string > timeList
- · DataSet ds
- int numberOfClusters = -1
- int extractOption = -1
- int maxIteration = -1
- bool isPBF
- bool isPathlines
- · int initialOption
- bool useTwoStage

4.1.1 Detailed Description

Definition at line 48 of file AffinityPropagation.h.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 AffinityPropagation::AffinityPropagation ()

Definition at line 11 of file AffinityPropagation.cpp.

```
12 {
13
14 }
```

4.1.2.2 AffinityPropagation::AffinityPropagation (const int & argc, char ** argv, const Para & p, bool & automatic)

Definition at line 29 of file AffinityPropagation.cpp.

```
30 {
       // set the data set information from the provided data set string name
32
       setDataset(argc, argv);
34
      if(automatic)
                      // automate the parameter setting
35
           setParameterAutomatic(p);
36
37
               // manually input the parameter
          getParameterUserInput();
39
40
      /\star select how to initialize the matrixS elements with preference value \star/
      std::cout << "Please select a MatrixS initialization? 1.median value, 2.minimal value (recommended!)."
41
      << std::endl;
std::cin >> initialOption;
42
43
       assert(initialOption==1||initialOption==2);
44 }
```

4.1.2.3 AffinityPropagation::~AffinityPropagation ()

Definition at line 53 of file AffinityPropagation.cpp.

```
54 {
55     // clear the cache memory for distance matrix
56     deleteDistanceMatrix(ds.dataMatrix.rows());
57 }
```

4.1.3 Member Function Documentation

4.1.3.1 void AffinityPropagation::clusterByNorm (const int & norm) [private]

Definition at line 129 of file AffinityPropagation.cpp.

```
130 {
131
        \ensuremath{//} The parameters to record time needed for calculation
132
        struct timeval start, end;
133
        double timeTemp;
134
135
        // calculate the distance matrix given the similarity measure type
136
        getDistanceMatrixFromFile(norm);
137
138
        Eigen::MatrixXf matrixR, matrixA, matrixS;
139
140
        gettimeofday(&start, NULL);
141
142
        /*-----/First-level Affinity Propagation-----*/
143
144
        // perform the AP clustering based on given distance matrix and matrix S, R and A
        performAPClustering(matrixS, matrixR, matrixA, distanceMatrix,
145
      ds.dataMatrix);
146
147
        \ensuremath{//} calculate and record the time for first-level AP clustering
148
        gettimeofday(&end, NULL);
149
        timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u+ end.tv_usec - start.tv_usec) / 1.e6;
150
151
        activityList.push_back("First-level affinity propagation takes: ");
152
        timeList.push_back(to_string(timeTemp)+" s");
153
        // some parameters for two-level AP clustering algorithm
154
        std::vector<std::vector<int> > neighborVec;
155
        std::vector<int> storage;
156
157
        Eigen::MatrixXf centroid;
158
159
        // get exemplary examples from the first-level {\ensuremath{\mathtt{AP}}}
160
        getGroupAssignment(matrixR, matrixA, matrixS, neighborVec, storage,
      group);
161
        // set the labels of initial samples by first-level AP
162
163
        setLabel(neighborVec, storage, centroid, group);
164
        activityList.push_back("First-level affinity propagation generates: ");
timeList.push_back(to_string(storage.size())+" groups");
165
166
167
168
        if(useTwoStage) // two-staged AP is activated
169
170
171
        /*----Second-level Affinity Propagation ------
172
         * Use the centroid of the first level and then apply affinipty propagation once again -----
173
174
            gettimeofday(&start, NULL);
175
176
             /\star get distance matrix for the centroids \star/
177
            float ** centroidDistMatrix = NULL;
            getDistMatrixForCentroids(&centroidDistMatrix,
178
      normOption, centroid);
179
180
             // perform second-level Affinity Propagation on centroids of the streamlines/pathlines
181
            performAPClustering(matrixS, matrixR, matrixA, centroidDistMatrix, centroid);
182
        // release the memory of centroidDistMatrix
#pragma omp parallel for schedule(static) num_threads(8)
183
184
185
            for(int i=0; i<centroid.rows(); ++i)</pre>
186
```

```
187
                 delete[] centroidDistMatrix[i];
                 centroidDistMatrix[i] = NULL;
188
189
190
             delete[] centroidDistMatrix;
191
             centroidDistMatrix = NULL;
192
193
             // record the time into the README
194
             gettimeofday(&end, NULL);
            timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u+ end.tv_usec - start.tv_usec) / 1.e6;
activityList.push_back("Second-level affinity propagation takes: ");
timeList.push_back(to_string(timeTemp)+" s");
195
196
197
198
199
             /* extract the group information */
200
             std::vector<std::vector<int> > secondNeighborVec;
201
             std::vector<int> secondStorage;
202
             Eigen::MatrixXf secondCentroid;
203
204
             std::vector<int> centroidGroup(centroid.rows());
205
206
             /* get exemplary examples */
             getGroupAssignment(matrixR, matrixA, matrixS, secondNeighborVec, secondStorage,
207
      centroidGroup);
208
             // get the label of each candidate lines by two-level AP clustering
209
210
             setLabel(secondNeighborVec, secondStorage, secondCentroid, centroidGroup);
211
212
             secondNeighborVec.clear();
213
214
            // record the consumed time
             activityList.push_back("Second-level affinity propagation generates: ");
timeList.push_back(to_string(secondStorage.size())+" groups");
215
216
218
                    219
             \ensuremath{//} should re-calculate the centroid, storage and neighborVec for new clusters
             getHierarchicalClusters(storage, neighborVec, centroid,
220
      group, centroidGroup, secondStorage.size());
221
222
223
         // begin to calculate the evaluation metrics and cluster representatives
224
        extractFeatures(storage, neighborVec, centroid);
225
226 }
```

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

Definition at line 301 of file AffinityPropagation.cpp.

```
303 {
304
                             const int& Row = ds.dataMatrix.rows();
const int& Column = ds.dataMatrix.cols();
305
306
307
                              /* record labeling information */
308
                             // IOHandler::generateGroups(neighborVec);
309
                             // Output the number of candidates inside each streamline cluster std::cout << "Final group number information: " << std::endl; for (int i=0; i < storage.size(); ++i)
310
311
312
313
314
                                             std::cout << storage[i] << " ";
315
316
                             std::cout << std::endl;
317
318
                              // calculate the normalized entropy to check the balance of cluster size
319
                              float EntropyRatio;
320
                             getEntropyRatio(storage, EntropyRatio);
321
322
                              // print the cluster labels in the primary .vtk file
323
                             {\tt IOHandler::printClusters\,(ds.dataVec,group,storage,"AP\_norm"+to\_string\,(ds.dataVec,group,storage,"approximation and approximation of the printClusters and approximation 
                      normOption), ds.fullName, ds.dimension);
324
325
                              struct timeval start, end;
326
                              double timeTemp;
327
328
                              /* compute the centroid coordinates of each clustered group */
329
330
                             gettimeofday(&start, NULL);
331
```

```
332
        vector<vector<float> > closest(numberOfClusters);
333
        vector<vector<float> > furthest(numberOfClusters);
334
335
        /\star extract the closest and furthest streamlines to centroid \star/
336 #pragma omp parallel for schedule(static) num_threads(8)
        for (int i=0;i<numberOfClusters;++i)</pre>
337
338
339
            float minDist = FLT_MAX;
            float maxDist = -10;
int minIndex = -1, maxIndex = -1;
340
341
            const std::vector<int>& groupRow = neighborVec[i];
342
            const Eigen::VectorXf& eachCentroid = centroid.row(i);
343
344
            for (int j = 0; j < groupRow.size(); ++j)
345
346
                float distance = getDisimilarity(eachCentroid, ds.dataMatrix, groupRow[j],
      normOption,object);
347
                if (minDist>distance)
348
                {
349
                    minDist = distance;
350
                    minIndex = groupRow[j];
351
352
                if (maxDist<distance)
353
                    maxDist = distance:
354
                    maxIndex = groupRow[j];
355
356
357
358
            closest[i] = ds.dataVec[minIndex];
359
            furthest[i] = ds.dataVec[maxIndex];
360
        }
361
        // convert the centroid matrix into vector<vector<float>> type. It is not necessary actually
362
        std::vector<std::vector<float> > center_vec(numberOfClusters, vector<float>(Column));
363
364 #pragma omp parallel for schedule(static) num_threads(8)
365
        for (int i = 0; i < center_vec.size(); ++i)</pre>
366
367
            for (int j = 0; j < Column; ++j)
368
369
                center_vec[i][j] = centroid(i,j);
370
371
372
373
        \ensuremath{//} Record the time for extracting the cluster representative lines
374
        gettimeofday(&end, NULL);
        timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u
375
376
                  + end.tv_usec - start.tv_usec) / 1.e6;
377
        activityList.push_back("Feature extraction takes: ");
        timeList.push_back(to_string(timeTemp)+" s");
378
379
380
        // calculate the normalized validity measurement metric for clustering evaluation
381
        ValidityMeasurement vm;
        vm.computeValue(normOption, ds.dataMatrix, group, object,
382
      isPBF);
383
        activityList.push_back("Validity measure is: ");
384
        stringstream fc_ss;
385
        fc ss << vm.f c;
        timeList.push_back(fc_ss.str());
386
387
388
        std::cout << "Finishing extracting features!" << std::endl;</pre>
389
        // calculate silhouette, the Gamma statistics and DB index for clustering evaluation
390
391
        gettimeofday(&start, NULL);
392
        Silhouette sil;
        sil.computeValue(normOption, ds.dataMatrix, ds.
393
      dataMatrix.rows(),ds.dataMatrix.cols(),group,object,
394
                         numberOfClusters, isPBF, neighborVec);
        395
396
397
        activityList.push_back("Silhouette calculation takes: ");
398
399
        timeList.push_back(to_string(timeTemp)+" s");
400
        stringstream ss;
ss << "norm_" << normOption;</pre>
401
402
403
404
        /* measure closest and furthest rotation */
405
        std::vector<float> closestRotation, furthestRotation;
406
        const float& closestAverage = getRotation(closest, closestRotation);
407
        const float& furthestAverage = getRotation(furthest, furthestRotation);
408
409
        /\star save closest, furthest and centroid representative streamlines \star/
        IOHandler::printFeature(ds.dataName+"_AP_closest_"+ss.str()+".vtk", closest, sil.sCluster,
410
                closestRotation, ds.dimension);
411
412
        IOHandler::printFeature(ds.dataName+"_AP_furthest_"+ss.str()+".vtk", furthest, sil.sCluster,
413
                furthestRotation, ds.dimension);
        IOHandler::printFeature(ds.dataName+"_AP_centroid_"+ss.str()+".vtk", center_vec, sil.sCluster
414
      .ds.dimension):
```

```
415
         IOHandler::printToFull(ds.dataVec, sil.sData, "AP_SValueLine_"+ss.str(),
416
      ds.fullName, ds.dimension);
417
        IOHandler::printToFull(ds.dataVec, group, sil.sCluster, "AP_SValueCluster_"+ss.str(),
      ds.fullName, ds.dimension);
418
         // record the clustering evaluation metric values in the txt file activityList.push_back("numCluster is: ");
419
420
421
         timeList.push_back(to_string(numberOfClusters));
422
         activityList.push_back("Norm option is: ");
423
         timeList.push_back(to_string(normOption));
424
425
426
         IOHandler::generateReadme(activityList,timeList);
427
         /* print entropy value for the clustering algorithm */
IOHandler::writeReadme(EntropyRatio, sil, "For norm "+to_string(normOption));
428
429
430
431
         IOHandler::writeReadme(closestAverage, furthestAverage);
432 }
```

4.1.3.3 void AffinityPropagation::getDistanceMatrixFromFile (const int & norm) [private]

Definition at line 870 of file AffinityPropagation.cpp.

```
871 {
        normOption = norm;
872
873
874
         /\star very hard to decide whether needed to perform such pre-processing, but recommended
875
         * to create a cached object for further pair-wise distance matrix calculation
876
877
        object = MetricPreparation(ds.dataMatrix.rows(), ds.dataMatrix.cols());
878
        object.preprocessing(ds.dataMatrix, ds.dataMatrix.rows(),
      ds.dataMatrix.cols(), normOption);
879
880
         /\star would store distance matrix instead because it would save massive time \star/
881
         struct timeval start, end;
882
        double timeTemp;
883
        gettimeofday(&start, NULL);
884
885
            in case the distance matrix already exists for other similarity, will clean it first
886
        deleteDistanceMatrix(ds.dataMatrix.rows());
887
888
         // read distance matrix from the local file in ../dataset/
889
        std::ifstream distFile(("../dataset/"+to_string(normOption)).c_str(), ios::in);
890
891
         // the local file of distance matrix does not exist, then will create the file
892
         if (distFile.fail())
893
894
             distFile.close();
895
             \ensuremath{//} calculate the distance matrix from norm option
             getDistanceMatrix(ds.dataMatrix, normOption, object);
std::ofstream distFileOut(("../dataset/"+to_string(normOption)).c_str(), ios::out);
896
897
898
             for (int i=0; i < ds.dataMatrix.rows(); ++i)</pre>
899
900
                  for(int j=0; j<ds.dataMatrix.rows();++j)</pre>
901
                      distFileOut << distanceMatrix[i][j] << " ";</pre>
902
903
904
                 distFileOut << std::endl;
905
906
             distFileOut.close();
907
908
        else // the local file for distance matrix computation exists, then directly read in
909
910
             std::cout << "read distance matrix..." << std::endl;
911
912
              // create the distance matrix and read in the content
         distanceMatrix = new float*[ds.dataMatrix.rows()];
#pragma omp parallel for schedule(static) num_threads(8)
913
914
915
             for (int i = 0; i < ds.dataMatrix.rows(); ++i)</pre>
916
             {
917
                 distanceMatrix[i] = new float[ds.dataMatrix.rows()];
918
919
             int i=0,
920
             string line;
921
             stringstream ss;
922
             // extract the distance values from the file
923
             while (getline (distFile, line))
924
```

```
j=0;
                  ss.str(line);
926
927
                  while (ss>>line)
928
                  {
                       <u>if</u>(i==j)
929
930
                            distanceMatrix[i][i]=0;
931
                       else
932
                            distanceMatrix[i][j] = std::atof(line.c_str());
933
934
                  ++i;
935
                  ss.str("");
936
937
                  ss.clear();
938
939
              distFile.close();
940
941
942
         gettimeofday(&end, NULL);
         timeTemp = ((end.tv_sec - start.tv_sec) * 1000000u
+ end.tv_usec - start.tv_usec) / 1.e6;
943
944
      activityList.push_back("Distance matrix computing for norm "+to_string(
normOption)+" takes: ");
945
946
         timeList.push_back(to_string(timeTemp)+" s");
947 }
```

4.1.3.4 void AffinityPropagation::getDistMatrixForCentroids (float *** centroidDistMatrix, const int & norm, const Eigen::MatrixXf & centroid) [private]

Definition at line 838 of file AffinityPropagation.cpp.

```
840 {
841
         const int& rows = centroid.rows();
842
         *centroidDistMatrix = new float*[rows];
843
844
         /\star in order to calculate the distance matrix given norm, we need to calculate the object first. This
       object
845
          * is to pre-calculate some preliminary stuff for distance matrix computation. I know it is redundant
       but in
846
         * practice it can help to accelerate the performance a little bit
847
848
849
         MetricPreparation centroidObj = MetricPreparation(centroid.rows(), centroid.cols());
850
         centroidObj.preprocessing(centroid, centroid.rows(), centroid.cols(), norm);
851
852 // calculate the distance matrix among centroid matrix coordinates
853 #pragma omp parallel for schedule(static) num_threads(8)
854 for(int i=0; i<rows; ++i)
855
856
              (*centroidDistMatrix)[i] = new float[rows];
857
             for(int j=0; j<rows; ++j)</pre>
858
                  (*centroidDistMatrix)[i][j] = getDisimilarity(centroid, i, j, norm, centroidObj);
859
860
             }
         }
862 }
```

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

Definition at line 485 of file AffinityPropagation.cpp.

```
486 {
487
        // the formula is -s[i]/S * log(s[i]/S), and then normalized by log(numOfClusters)
488
        EntropyRatio = 0;
489
        const int& Row = ds.dataMatrix.rows();
490
        for (int i = 0; i < storage.size(); ++i)</pre>
491
492
            float ratio = float(storage[i])/float(Row);
493
            EntropyRatio-=ratio*log2f(ratio);
494
        /\star the higher value shows that the final clusters are balanced and almost equal sized, while the
495
496
            low value shows the contrary
497
498
        EntropyRatio/=log2f(storage.size());
499 }
```

4.1.3.6 void AffinityPropagation::getGroupAssignment (const Eigen::MatrixXf & matrixA, const Eigen::MatrixXf & matrixA, const Eigen::MatrixXf & matrixS, std::vector< int > & neighborVec, std::vector< int > & storage, std::vector< int > & groupTag) [private]

Definition at line 757 of file AffinityPropagation.cpp.

```
760 {
         std::vector<int> centerVec;
762
        const int& rows = matrixR.rows();
763
764
         /\star store the candidate whose diagonal summation is positive \star/
765
        float diagonalSum;
766
         for(int i=0;i<rows;++i)</pre>
767
768
             diagonalSum=matrixR(i,i)+matrixA(i,i);
769
             if(diagonalSum>0)
770
771
                 centerVec.push_back(i);
772
773
774
         const int& centerSize = centerVec.size();
775
776 /* get group tag information for each candidate streamline */ 777 #pragma omp parallel for schedule(static) num_threads(8)
778
         for(int i=0;i<rows;++i)</pre>
779
780
             int index, element;
781
             float maxSim = -FLT_MAX;
782
             for(int j=0;j<centerSize;++j)</pre>
783
784
                 element = centerVec[i];
785
                 if (matrixS(i,element)>maxSim)
786
787
                      maxSim = matrixS(i,element);
788
                      index = element;
789
790
791
             groupTag[i]=index;
792
793
         /* output group information and cluster size */
794
795
         std::map<int,int> groupMap;
796
         for(int i=0;i<rows;++i)</pre>
797
798
             /* group tag not int the hash map */
799
             if(groupMap.find(groupTag[i]) == groupMap.end())
800
801
                  groupMap.insert(make_pair(groupTag[i],0));
802
803
804
805
         /\star give them new index starting from 0 \star/
806
807
         for(auto iter = groupMap.begin();iter!=groupMap.end();++iter)
808
809
             iter->second = count++:
810
811
        numberOfClusters = groupMap.size();
813
814
         /* assign contained element and size */
815
        neighborVec = std::vector<std::vector<int> > (numberOfClusters);
816
        storage = std::vector<int>(numberOfClusters);
817
         for (int i=0; i < rows; ++i)</pre>
818
819
             count = groupMap[group[i]];
820
             neighborVec[count].push_back(i);
821
822
         /* assign the storage vector */
824
         for(int i=0;i<storage.size();++i)</pre>
825
826
             storage[i] = neighborVec[i].size();
827
828 }
```

4.1.3.7 void AffinityPropagation::getHierarchicalClusters (std::vector< int > & storage, std::vector< std::vector< int > > & neighborVec, Eigen::MatrixXf & centroid, std::vector< int > & group, const std::vector< int > & centroidGroup, const int & groupSize) [private]

Definition at line 993 of file AffinityPropagation.cpp.

```
996 {
        neighborVec.clear();
997
998
        neighborVec.resize(groupSize);
999
        storage.resize(groupSize);
1000
         centroid = Eigen::MatrixXf::Zero(groupSize, centroid.cols());
1001
1002
         int groupID;
1003
         for(int i=0; i<groupTag.size(); ++i)</pre>
1004
1005
             groupID = centroidGroup[groupTag[i]];
             groupTag[i] = groupID;
1006
1007
             neighborVec[groupID].push_back(i);
1008
             centroid.row(groupID)+=ds.dataMatrix.row(i);
1009
1010
1011 #pragma omp parallel for schedule(static) num_threads(8)
1012
         for(int i=0; i<groupSize; ++i)</pre>
        {
1013
1014
             centroid.row(i)/=neighborVec[i].size();
             storage[i] = neighborVec[i].size();
1016
1017 }
```

4.1.3.8 void AffinityPropagation::getMatrixS (Eigen::MatrixXf & matrixS, float ** distMatrix, const Eigen::MatrixXf & coordinates) [private]

Definition at line 584 of file AffinityPropagation.cpp.

```
585 {
586
        std::cout << "Start initializing matrix S..." << std::endl;</pre>
587
588
        const int& rows = matrixS.rows();
589
        /\star define a vector to store pair-wise distance vector and get the median \star/
590
        const int& distVecSize = rows*(rows-1)/2;
591
592
        std::vector<float> distVec(distVecSize);
593
        int count = 0;
594
595
        /\star find the minimal dissimilarity value from the distance matrix \star/
596
        float minV = (float)FLT_MAX;
597
        float tempDist;
598
        for (int i=0; i < rows-1; ++i)</pre>
599
600
             for (int j=i+1; j<rows; ++j)</pre>
601
                 if(distMatrix) // if distance matrix exists, direct fetch the cached value
602
                     tempDist = distMatrix[i][j];
e    // otherwise, has to calculate the distance matrix
603
604
605
                      tempDist = getDisimilarity(coordinates, i, j, normOption, object);
606
607
                 /\star conventionally we assign -d*d as non-diagonal entries for matrix S \star/
                 matrixS(i,j) = -tempDist;
matrixS(j,i) = matrixS(i,j);
608
609
610
                 minV = std::min(minV, matrixS(i,j));
612
                 distVec[count++] = matrixS(i,j);
613
             }
614
615
616
        std::cout << "min Value is " << minV << std::endl;</pre>
617
        assert(count==distVecSize);
618
619
        float initialValue;
                                 // the initialization is by median of distance matrix values
620
        if(initialOption==1)
621
622
              ^{\prime}\star get median value to be assigned for S(i,i) \star/
623
             float medianValue, leftMedian, rightMedian;
624
625
             /\star odd size, just pick mid index \star/
             if (distVecSize%2==1)
626
                medianValue = select(distVec, 0, distVecSize-1, distVecSize/2);
627
628
             /\star even size, choose average of left and right \star/
629
             else if (distVecSize%2==0)
630
            {
631
                 leftMedian = select(distVec, 0, distVecSize-1, (distVecSize-1)/2);
632
                 rightMedian = select(distVec, 0, distVecSize-1, distVecSize/2);
633
                 medianValue = (leftMedian+rightMedian)/2.0;
634
             // assign the preference value as median of the distance matrix values
```

```
initialValue = medianValue;
637
638
        else if(initialOption==2) // the initialization is by minimal dissimilarity value
639
640
             initialValue = minV:
641
        std::cout << "Initial value is " << initialValue << std::endl;</pre>
642
643
644
        /* assign the initialValue to diagonal matrix element */
645 #pragma omp parallel for schedule(static) num_threads(8)
646 for(int i=0;i<rows;++i)
647
            matrixS(i,i) = initialValue;
648
649
        std::cout << "Finish initializing matrix S..." << std::endl;</pre>
650 }
```

4.1.3.9 void AffinityPropagation::getParameterUserInput() [private]

Definition at line 541 of file AffinityPropagation.cpp.

```
542 {
        // User input for streamline/pathline sampleOption
543
544
        int sampleOption;
        std::cout << "choose a sampling method for the dataset?" << std::endl</pre>
545
546
                  << "1.directly filling with last vertex; 2. uniform sampling." << std::endl;
547
        std::cin >> sampleOption;
548
        assert(sampleOption==1||sampleOption==2);
549
        if(isPathlines) // if is pathlines, directly repeat the last vertex of pathlines
550
551
            IOHandler::expandArray(ds.dataMatrix, ds.dataVec, ds.
      dimension, ds.maxElements);
552
               // for streamlines, there are multiple options for that
553
            if(sampleOption==1) // direct repeat the last vertex
554
                IOHandler::expandArray(ds.dataMatrix,ds.dataVec,
555
      ds.dimension, ds.maxElements);
    else if (sampleOption==2)
                                         // sample the array on the intervals
                IOHandler::sampleArray(ds.dataMatrix,ds.dataVec,
557
      ds.dimension,ds.maxElements);
558
        else if(sampleOption==3)
                                         // sample the array with equal arc
                IOHandler::uniformArcSampling(ds.dataMatrix,ds.dataVec,
559
      ds.dimension,ds.maxElements);
560
561
562
        group = std::vector<int>(ds.dataMatrix.rows());
563
        // select cluster represnetative strategy, and 1 is recommended
564
        std::cout << "Select extraction method: 1.centroid, closest and furthest (recommended!), 2.median."
565
566
                << std::endl;
567
        std::cin >> extractOption;
568
        assert(extractOption==1||extractOption==2);
569
570
        // Input the maximal iteration for AP clustering algorithm
571
        std::cout << "Input max iteration for affinity propagation: " << std::endl;</pre>
572
        std::cin >> maxIteration;
        assert(maxIteration>0);
574 }
```

4.1.3.10 void AffinityPropagation::initializeMatrices (Eigen::MatrixXf & matrixS, Eigen::MatrixXf & matrixR, Eigen::MatrixXf & matrixA, const int & rows) [private]

Definition at line 661 of file AffinityPropagation.cpp.

```
663 {
664     /* initialize all three matrices as zero entry */
665     matrixS = Eigen::MatrixXf::Zero(rows, rows);
666     matrixR = Eigen::MatrixXf::Zero(rows, rows);
667     matrixA = Eigen::MatrixXf::Zero(rows, rows);
668 }
```

4.1.3.11 void AffinityPropagation::performAPClustering (Eigen::MatrixXf & matrixS, Eigen::MatrixXf & matrixAf, float ** distMatrix, const Eigen::MatrixXf & coordinates) [private]

Definition at line 959 of file AffinityPropagation.cpp.

```
961 {
962
        /* initialize S, R, A */
963
        initializeMatrices(matrixS, matrixR, matrixA, coordinates.rows());
964
965
966
        getMatrixS(matrixS, distMatrix, coordinates);
967
968
        int current = 0:
969
        while (current++<maxIteration)</pre>
970
971
            std::cout << "Iteration " << current << std::endl;</pre>
972
973
            /* update responsibility */
974
            updateResponsibility(matrixR, matrixA, matrixS);
975
976
            /* update availability */
977
            updateAvailability(matrixA, matrixR);
978
979
980 }
```

4.1.3.12 void AffinityPropagation::performClustering ()

Definition at line 67 of file AffinityPropagation.cpp.

```
68 {
69
        //distance metric type
70
       /* 0: Euclidean Norm, d(a,b) = (\sum_{a=b}^{\infty} (a-b)^2)^{(1/2)}.
71
            1: Fraction Distance Metric, d(a,b) = (\sum_{a=0}^{b} (a-b)^p)^(1/p), we choose p==0.5
72
           2: piece-wise angle average, from http://www2.cs.uh.edu/~chengu/Publications/3DFlowVis/
      curveClustering.pdf
73
           3: Bhattacharvva metric for rotation
            4: average rotation
75
           5: signed-angle intersection
76
            6: normal-direction multivariate distribution
           7: Bhattacharyya metric with angle to a fixed direction 8: Piece-wise angle average \landtimes standard deviation
77
78
            9: normal-direction multivariate un-normalized distribution
79
80
            10: x*v/|x||v| borrowed from machine learning
            11: cosine similarity
            12: Mean-of-closest point distance (MCP)
83
            13: Hausdorff distance min_max(x_i,y_i)
            14: Signature-based measure from http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6231627
84
            15: Procrustes distance take from http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6787131 16: entropy-based distance metric taken from http://vis.cs.ucdavis.edu/papers/pg2011paper.pdf
85
86
             17: time-series MCP distance from https://www.sciencedirect.com/science/article/pii/
      S0097849318300128
88
                 for pathlines only
89
90
       for (int i=0; i<=17; ++i)</pre>
91
            if(isPathlines) // for pathlines, it will call similarity measure d_T (17)
94
95
                 if(i!=0 && i!=1 && i!=2 && i!=4 && i!=12 && i!=13 && i!=14 && i!=15 && i!=17)
96
                     continue;
98
                   // for streamlines, d_T (17) will not be involved
            else
99
                  /* don't want to deal with many too naive metrics */ if(i!=0 && i!=1 && i!=2 && i!=4 && i!=12 && i!=13 && i!=14 && i!=15)
100
101
102
                      continue:
103
104
105
            std::cout << "-----
106
             std::cout << "Experiment on norm" << i << " starts!----- << std::endl;
107
108
             // clear out the recorded string information
109
             activityList.clear();
110
             timeList.clear();
111
```

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

Definition at line 441 of file AffinityPropagation.cpp.

```
442 {
443
        // the argc should be 3, e.g., ./ap cylinder 3
444
        if (argc!=3)
445
446
             std::cout << "Input argument should have 3!" << endl</pre>
                        << "./cluster inputFile_name(in dataset folder) "
447
448
                        << "data_dimension(3)" << endl;
449
             exit(1);
450
451
452
        // extract the required information from argument string
453
        ds.strName = string("../dataset/")+string(argv[1]);
454
        ds.dataName = string(argv[1]);
455
        ds.dimension = atoi(argv[2]);
456
        /* get the bool tag for variable isPBF */ std::cout << "It is a PBF dataset? 1.Yes, 0.No" << std::endl;
457
458
459
        int PBFjudgement;
460
        std::cin >> PBFjudgement;
461
        assert(PBFjudgement==1||PBFjudgement==0);
462
        isPBF = (PBFjudgement==1);
463
464
        /* check whether it is a Pathline data set or not */
        std::cout << "It is a Pathline? 1.Yes, 0. No" << std::endl;
465
466
        std::cin >> PBFjudgement;
467
        assert(PBFjudgement==1||PBFjudgement==0);
468
        isPathlines = (PBFjudgement==1);
469
470
        // read from the file into the member variables
        IOHandler::readFile(ds.strName, ds.dataVec, ds.vertexCount,
471
      ds.dimension,ds.maxElements);
472
473
        // print the streamline/pathline vtk file
        ds.fullName = ds.strName+"_full.vtk";
IOHandler::printVTK(ds.fullName, ds.dataVec, ds.
474
475
      vertexCount, ds.dimension);
476 }
```

4.1.3.14 void AffinityPropagation::setLabel (vector< vector< int > > & neighborVec, vector< int > & storage, Eigen::MatrixXf & centroid, std::vector< int > & groupTag) [private]

Definition at line 241 of file AffinityPropagation.cpp.

```
243 {
244
        // record the pair {cluster size, cluster candidate index}
245
        std::vector<Ensemble> nodeVec;
246
247
        for(int i=0;i<storage.size();++i)</pre>
248
249
            if(storage[i]==0)
250
            nodeVec.push_back({storage[i], neighborVec[i]});
251
252
253
254
        numberOfClusters = nodeVec.size();
255
256
        std::cout << "Cluster label setting begins with " << nodeVec.size() << " clusters..." << std::endl;
2.57
258
        /\star sort group index by size of elements containd inside to make sure that, 0 cluster has the
259
         * smallest size of candidates
260
```

```
261
        std::sort(nodeVec.begin(), nodeVec.end(), [](const Ensemble& first, const
      Ensemble& second)
{return first.size<second.size|| (first.size==second.size&first.</pre>
262
      element[0] < second.element[0]); });</pre>
263
264
        // re-define the neighborVec, storage and centroid coordinates given the new cluster index
        neighborVec = std::vector<std::vector<int> >(nodeVec.size());
265
        storage = std::vector<int>(nodeVec.size());
266
267
        centroid = Eigen::MatrixXf(nodeVec.size(), ds.dataMatrix.cols());
268
269
        // re-calculate the coordinates of the cluster centroids
270 #pragma omp parallel for schedule(static) num_threads(8)
271
        for(int i=0;i<nodeVec.size();++i)</pre>
272
273
            neighborVec[i] = nodeVec[i].element;
274
             storage[i] = nodeVec[i].size;
275
            Eigen::VectorXf tempVec = Eigen::VectorXf::Zero(ds.dataMatrix.cols());
276
            for(int j=0;j<storage[i];++j)</pre>
278
                 tempVec+=ds.dataMatrix.row(i).transpose();
279
                 /* don't forget to re-compute the group tag */
280
                 groupTag[neighborVec[i][j]]=i;
281
            centroid.row(i) = tempVec/storage[i];
282
283
285
        std::cout << "Cluster label setting ends..." << std::endl;</pre>
286 }
```

4.1.3.15 void AffinityPropagation::setParameterAutomatic (const Para & p) [private]

Definition at line 507 of file AffinityPropagation.cpp.

```
508 {
509
         // if the data set is pathline, will direct expand the array on the back
         if(isPathlines)
510
             IOHandler::expandArray(ds.dataMatrix,ds.dataVec,ds.
511
      dimension, ds.maxElements);
512
        else
                 // it is streamline
513
514
              if(p.sampled==1) // sampling is to directly expand the array from the back
      IOHandler::expandArray(ds.dataMatrix,ds.dataVec,
ds.dimension,ds.maxElements);
515
516
             else if(p.sampled==2)
                                           // sample the array on the intervals without change of geometric
517
                  IOHandler::sampleArray(ds.dataMatrix,ds.dataVec,
       ds.dimension,ds.maxElements);
        else if(p.sampled==3) // sample the array with equal arc
IOHandler::uniformArcSampling(ds.dataMatrix,ds.dataVec,
518
                                           \ensuremath{//} sample the array with equal arcs such that
519
      ds.dimension,ds.maxElements);
520
521
522
         // ceate a label vector for each candidate line
523
        group = std::vector<int>(ds.dataMatrix.rows());
524
525
         \ensuremath{//} assign the parameters for AP clustering
526
         extractOption = p.extractOption;
527
         maxIteration = p.maxIteration;
528
         /* whether to activate two-staged AP or not, see Jun Tao FlowString TVCG 2016 paper for details \star/ std::cout << "Whether to activate two-staged AP or not? 1.Yes, 2.No," << std::endl;
529
530
531
         int twoStageOption;
         std::cin >> twoStageOption;
533
         assert(twoStageOption==1 || twoStageOption==2);
534
         useTwoStage = (twoStageOption==1);
535 }
```

4.1.3.16 void AffinityPropagation::updateAvailability (Eigen::MatrixXf & matrixA, const Eigen::MatrixXf & matrixR)

[private]

Definition at line 709 of file AffinityPropagation.cpp.

```
710 {
        const int& rows = matrixR.rows();
711
712 #pragma omp parallel for schedule(static) num_threads(8)
713
        for(int i=0;i<rows;++i)</pre>
714
715
             for (int k=0; k<rows; ++k)
716
717
                 /\star for diagonal matrix, update by summation of non-diagonal entries in the row \star/
718
                 if(i==k)
719
720
                      float summation = 0.0;
721
                      for (int ii=0; ii<rows; ++ii)</pre>
722
723
724
                              continue;
725
                          summation+=std::max((float)0.0, matrixR(ii,k));
726
727
728
                      /* smoothing update instead of direct assignment */
729
                     matrixA(i,k) = (1-LAMBDA) *summation+LAMBDA*matrixA(i,k);
730
731
732
733
                      float summation = 0.0;
734
                      for(int ii=0;ii<rows;++ii)</pre>
735
736
                          if (ii==i||ii==k)
                              continue;
737
                          \verb|summation+=std::max((float)0.0, matrixR(ii,k));|\\
738
739
                     matrixA(i,k)=(1-LAMBDA)*std::min((float)0.0, matrixR(k,k)+summation)+
740
      LAMBDA*matrixA(i,k);
741
742
743
        }
744 }
```

4.1.3.17 void AffinityPropagation::updateResponsibility (Eigen::MatrixXf & matrixR, const Eigen::MatrixXf & matrixA, const Eigen::MatrixXf & matrixA) [private]

Definition at line 678 of file AffinityPropagation.cpp.

```
680 {
681
        const int& rows = matrixR.rows();
682
         // update the R with relaxed value of S and R
683 #pragma omp parallel for schedule(static) num_threads(8)
684
        for(int i=0;i<rows;++i)</pre>
685
686
             for (int k=0; k<rows; ++k)</pre>
687
                 /* don't use FLT_MIN because FLT_MIN == 0.0 */float maxValue = -FLT_MAX;
688
690
                  for(int kk=0;kk<rows;++kk)</pre>
691
692
                      if(kk==k)
693
                           continue:
694
                      maxValue = std::max(maxValue, matrixS(i,kk)+matrixA(i,kk));
695
696
                  /\star in wikipage it's update by R[i,k] = S[i][k]-maxValue, but here use a Laplace smoothor for
       convergence */
697
                 matrixR(i,k) = (1-LAMBDA) * (matrixS(i,k)-maxValue) + LAMBDA * matrixR(i,k);
698
699
        }
700 }
```

4.1.4 Member Data Documentation

4.1.4.1 std::vector<string> AffinityPropagation::activityList [private]

Definition at line 113 of file AffinityPropagation.h.

```
4.1.4.2 DataSet AffinityPropagation::ds [private]
Definition at line 123 of file AffinityPropagation.h.
4.1.4.3 int AffinityPropagation::extractOption = -1 [private]
Definition at line 133 of file AffinityPropagation.h.
4.1.4.4 std::vector<int> AffinityPropagation::group [private]
Definition at line 108 of file AffinityPropagation.h.
4.1.4.5 int AffinityPropagation::initialOption [private]
Definition at line 153 of file AffinityPropagation.h.
4.1.4.6 bool AffinityPropagation::isPathlines [private]
Definition at line 148 of file AffinityPropagation.h.
4.1.4.7 bool AffinityPropagation::isPBF [private]
Definition at line 143 of file AffinityPropagation.h.
4.1.4.8 int AffinityPropagation::maxIteration = -1 [private]
Definition at line 138 of file AffinityPropagation.h.
4.1.4.9 int AffinityPropagation::normOption = -1 [private]
Definition at line 103 of file AffinityPropagation.h.
4.1.4.10 int AffinityPropagation::numberOfClusters = -1 [private]
Definition at line 128 of file AffinityPropagation.h.
4.1.4.11 MetricPreparation AffinityPropagation::object [private]
Definition at line 98 of file AffinityPropagation.h.
```

4.1.4.12 std::vector<**string**> **AffinityPropagation::timeList** [private]

Definition at line 118 of file AffinityPropagation.h.

4.1.4.13 bool AffinityPropagation::useTwoStage [private]

Definition at line 158 of file AffinityPropagation.h.

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

- AffinityPropagation.h
- AffinityPropagation.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 17 of file Predefined.h.

4.2.2 Member Data Documentation

4.2.2.1 Eigen::MatrixXf DataSet::dataMatrix

Definition at line 20 of file Predefined.h.

4.2.2.2 string DataSet::dataName

Definition at line 27 of file Predefined.h.

4.2.2.3 vector < vector < float > DataSet::dataVec

Definition at line 19 of file Predefined.h.

4.2.2.4 int DataSet::dimension = -1

Definition at line 23 of file Predefined.h.

4.2.2.5 string DataSet::fullName

Definition at line 26 of file Predefined.h.

4.2.2.6 int DataSet::maxElements = -1

Definition at line 21 of file Predefined.h.

4.2.2.7 string DataSet::strName

Definition at line 25 of file Predefined.h.

4.2.2.8 int DataSet::vertexCount = -1

Definition at line 22 of file Predefined.h.

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

· Predefined.h

4.3 Ensemble Struct Reference

#include <Predefined.h>

Public Attributes

- int size
- std::vector< int > element

4.3.1 Detailed Description

Definition at line 35 of file Predefined.h.

4.3.2 Member Data Documentation

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

Definition at line 38 of file Predefined.h.

4.3.2.2 int Ensemble::size

Definition at line 37 of file Predefined.h.

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

· Predefined.h

4.4 Para Struct Reference

#include <AffinityPropagation.h>

Public Attributes

- int sampled
- int extractOption
- int maxIteration

4.4.1 Detailed Description

Definition at line 31 of file AffinityPropagation.h.

4.4.2 Member Data Documentation

4.4.2.1 int Para::extractOption

Definition at line 38 of file AffinityPropagation.h.

4.4.2.2 int Para::maxIteration

Definition at line 41 of file AffinityPropagation.h.

4.4.2.3 int Para::sampled

Definition at line 35 of file AffinityPropagation.h.

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

· AffinityPropagation.h

Chapter 5

File Documentation

5.1 AffinityPropagation.cpp File Reference

```
#include "AffinityPropagation.h"
Include dependency graph for AffinityPropagation.cpp:
```

5.2 AffinityPropagation.h File Reference

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

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

Classes

- struct Para
- class AffinityPropagation

Macros

• #define LAMBDA 0.5

5.2.1 Macro Definition Documentation

5.2.1.1 #define LAMBDA 0.5

Definition at line 21 of file AffinityPropagation.h.

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5.3 main.cpp File Reference

```
#include "AffinityPropagation.h"
Include dependency graph for main.cpp:
```

Functions

- void setPara (Para &p)
- int main (int argc, char **argv)

5.3.1 Function Documentation

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

Definition at line 12 of file main.cpp.

```
13 {
14
       Para p;
15
16
       setPara(p);
17
18
       /\star enable automatic option \star/
19
       bool automatic = true;
20
21
       AffinityPropagation ap(argc, argv, p, automatic);
23
       ap.performClustering();
24
25
       return 0;
26 }
```

5.3.1.2 void setPara (Para & p)

Definition at line 33 of file main.cpp.

```
34 {
35     /* 1.directly filling with last vertex; 2. uniform sampling, 3. equal-arc sampling */
36     p.sampled = 2;
37
38     /* extraction option, 1. centroid, closest and furthest, 2. median, 3. statistical representation */
39     p.extractOption = 1;
40
41     /* max iteration for AP clustering */
42     p.maxIteration = 20;
43
44 }
```

5.4 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

Functions

```
template < class T > void mySwap (T &a, T &b)
```

• template<class T >

int partition (std::vector < T > & array, const int & left, const int & right, const int & pivotIndex)

template<class T >

T select (std::vector< T > &array, int left, int right, const int &k)

5.4.1 Function Documentation

```
5.4.1.1 template < class T > void mySwap ( T & a, T & b )
```

Definition at line 45 of file Predefined.h.

5.4.1.2 template < class T > int partition (std::vector < T > & array, const int & left, const int & right, const int & pivotIndex)

Definition at line 62 of file Predefined.h.

```
63 {
       T pivotValue = array[pivotIndex];
64
       mySwap(array[pivotIndex], array[right]);
65
       int storeIndex = left;
66
       for (int i=left; i<right;++i)</pre>
69
           if (array[i] < pivotValue)</pre>
70
                mySwap(array[storeIndex], array[i]);
71
                ++storeIndex:
73
75
       mySwap(array[right], array[storeIndex]);
76
77 }
       return storeIndex;
```

5.4.1.3 template < class T > T select (std::vector < T > & array, int left, int right, const int & k)

Definition at line 91 of file Predefined.h.

```
92 {
93
        int pivotIndex;
94
        while (true)
95
             if(left==right)
                  return array[left];
97
            pivotIndex = (left+right)/2;
pivotIndex = partition(array, left, right, pivotIndex);
98
99
100
             if(k==pivotIndex)
101
                  return array[k];
102
             else if(k<pivotIndex)</pre>
103
                  right = pivotIndex-1;
104
             else
105
                  left = pivotIndex+1;
106
         }
107 }
```

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5.5 README.md File Reference

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