

User Manual for AMVML

1. Method Description

AMVML(Adaptive Multi-View Multi-Label Learning) is a computational framework that can effectively and reliably uncover potential disease-related miRNAs. It learns a new affinity graph adaptively for both diseases and miRNAs from multiple biological data sources. It also simultaneously update the miRNA-disease association predicted from both miRNA and disease spaces based on multi-label learning. In particular, the convergence of AMVML has been proved theoretically and the corresponding analysis indicates that it has a fast convergence rate. It is also worth mentioning that AMVML can be easily extended if there are more biological datasets available.

2. Requirements

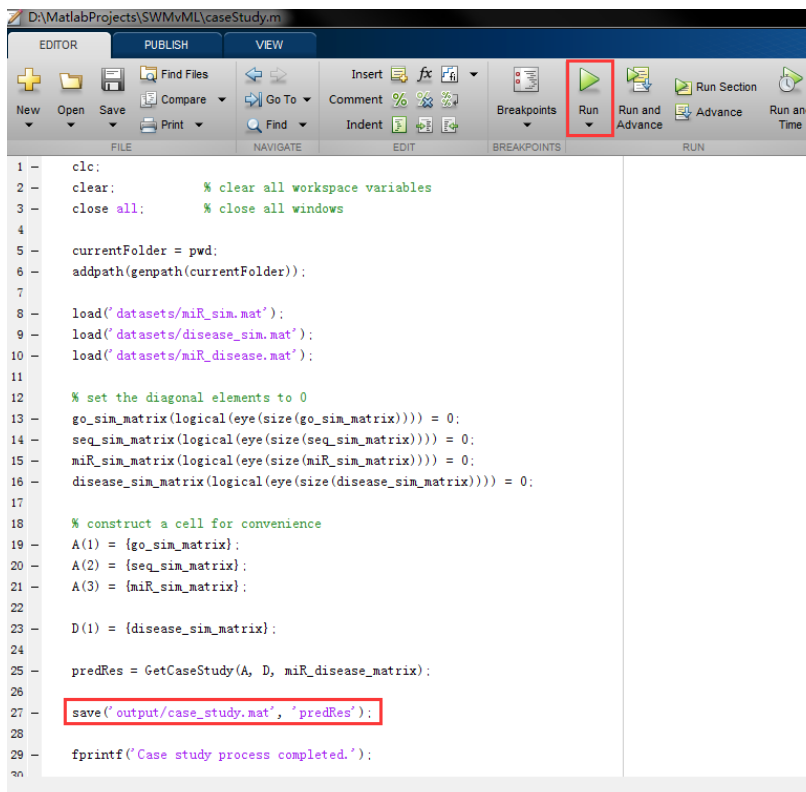
AMVML was developed in MATLAB 2014b environment and it should be compatible with all MATLAB versions.

3. Usage

We provided two functions, case study and global leave-one-out cross-validation (LOOCV), for users. All the datasets involved in the code, i.e. miRNA sequence similarity, miRNA functional similarity, miRNA semantic similarity, disease semantic similarity and miRNA-disease associations are all provided in 'datasets/*.mat'.

1) case study

To run the case study, please open the script 'caseStudy.m' into your MATLAB programming environment and click 'Run' as illustrated below:



The program should start to run immediately and it should be finishing in five minutes. Once the program finishes, the output of the case study results is saved at 'output/case_study.mat'. Users can change the output directory according to their own needs. The output of the case study is of the following format:

	1	2	3	4	5	6	7	8	9	10	11
1	0.9999	0.9997	0.9999	0.9999	0.9999	2.9122e-05	0.9999	3.7189e-06	0.9999	0.9997	0.9999
2	0.9999	0.9997	0.9999	0.9999	0.9999	3.9539e-05	0.9999	3.5474e-06	0.9999	1.6707e-04	0.9998
3	0.9999	1.8662e-04	0.9999	0.9999	0.9999	2.7465e-05	0.9999	2.3404e-06	0.9999	1.5549e-04	0.9998
4	0.9999	0.9997	0.9999	0.9999	0.9998	6.7244e-05	0.9999	2.3170e-06	0.9999	0.9997	1.6092e-04
5	0.9999	0.9997	0.9998	0.9999	0.9999	0.9997	0.9998	3.3839e-05	0.9999	0.9997	1.6013e-04
6	0.9998	0.9998	0.9999	0.9999	0.9999	7.5274e-05	0.9999	3.8533e-06	0.9999	0.9997	1.7368e-04
7	0.9999	0.9997	0.9998	0.9999	0.9999	0.9997	0.9998	3.3306e-05	0.9999	1.2838e-04	1.5783e-04
8	0.9998	0.9998	0.9998	0.9999	0.9999	6.9268e-05	0.9999	1.6031e-06	0.9999	1.1919e-04	0.9998
9	0.9998	0.9998	0.9998	0.9999	0.9999	6.6708e-05	0.9998	4.9214e-09	0.9999	1.1060e-04	0.9998
10	0.9999	1.7060e-04	0.9999	0.9999	0.9999	7.7823e-05	0.9999	7.1954e-06	0.9999	1.3976e-04	0.9998
11	0.9998	1.1778e-04	0.9998	0.9998	0.9998	0.9997	0.9998	3.6742e-05	0.9998	1.0610e-04	1.4059e-04
12	9.6677e-05	9.3932e-05	0.9999	2.8019e-04	0.9998	0.9997	0.9998	1.2238e-04	0.9998	0.9998	0.9998
13	0.9998	5.3954e-05	0.9999	0.9999	0.9999	2.7270e-05	0.9998	1.6387e-05	0.9998	0.9999	0.9998
14	1.2557e-04	6.8945e-05	0.9998	0.9998	0.9999	0.9998	0.9998	0.9998	0.9998	9.2266e-05	0.9998
15	1.3545e-04	7.7098e-05	0.9998	0.9999	0.9999	0.9998	0.9998	0.9998	0.9998	1.5556e-04	0.9998
16	0.9998	7.5856e-05	0.9998	0.9998	2.0810e-04	4.9782e-06	0.9998	1.5749e-06	0.9997	0.9997	0.9998
17	0.9997	0.9997	1.3709e-04	0.9998	0.9998	5.4415e-05	0.9998	4.2183e-05	1.1083e-04	0.9997	0.9998

Each entry in the matrix represents a predicted association probability of the corresponding miRNA-disease association. However, users should be aware that we only need to consider the predicted probability of unknown miRNA-disease associations.

Users can also run the script in standard command-line mode as shown below (suppose the current working directory is 'D:\MatlabProjects\SWMvML', it is also the same under LINUX environment):

```
D:\MatlabProjects\SWMvML>matlab -nodisplay -nodesktop -nosplash -r "caseStudy;exit;";
```

2) global LOOCV

Similarly, to run global LOOCV, please open the script 'global_loocv.m' accordingly and other operations are the same as that of case study. During each iteration, our algorithm will display the ranking of the current tested association and its corresponding predicted score as follows:

```
Command Window

Iteration stops at 8 step.
Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 1
Predicting score is  : 3.198898e-04
The current ranking is : 5.000000e-01

Iteration stops at 9 step.
Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 2
Predicting score is  : 3.029186e-04
The current ranking is : 1.500000e+00

Iteration stops at 10 step.
Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 3
Predicting score is  : 2.925097e-04
The current ranking is : 2
```

The output of the global LOOCV is of the following format:

	1	2	3	4	5	6	7	8	9	10	11
1	0.5000	1.5000	2	3.5000	2.5000	10	2	2.5000	3	2	13
2											
3											
4											
5											
6											
7											
8											

where each number, i.e. 0.5000, 1.5000, 2 and etc., represent the average ranking of the known miRNA-disease association tested in turn. The program can also be executed in standard command-line mode as follows:

```
D:\MatlabProjects\SVMvML>matlab -nodisplay -nodesktop -nosplash -r "global_loocv;exit;"
```

4. Parameters

There are two parameters α and β in AMVML that need to be predetermined by users. The default value for both parameters are $1e-4$. Users can change their value in "MultiViewPrediction.m" file as follows:

```
function [F] = MultiViewPrediction(AM, AD, Y)
% AD: the multi-view disease-disease similarity matrix
% AM: the multi-view miRNA-miRNA similarity matrix
% Y : the ground truth (the known miRNA-disease associations)
% F : the result predicted by our method

AMview = size(AM, 2);
ADview = size(AD, 2);

AMweight = 1 / AMview * ones(1, AMview);
ADweight = 1 / ADview * ones(1, ADview);

alpha = 0.0001;
beta = 0.0001;
gamma = 1;

NIITER = 15;
thresh = 10^-12; % Iterative terminating condition
```

To set appropriate values for these two parameters, please refer to the "Parameter Analysis" section in our paper.

5. Contact

For any questions regarding our work, please feel free to contact us: alcs417@sdnu.edu.cn