

User Manual for SwMKML

1. Method Description

We proposed a novel Self-weighted multi-kernel multi-label learning method for potential miRNA-disease associations prediction. We used multi-views, including several gaussian matrix calculated by gaussian kernel function and the miRNA functional similarity matrix as well as the disease semantic similarity matrix based on the latest version of MeSH descriptors and HMDD. We adopted an iterative and alternative optimization algorithm, and solved each of the variables separately by fixing other variables. Finally, the predicted miRNA-disease associations matrix was obtained by combining the miRNA space and disease space together. In particular, we proved the convergence of SwMKML algorithm through experiments and the corresponding analysis indicated that it had a fast convergence rate. It was also worth mentioning that SwMKML could be easily extended if there are more biological datasets available.

2. Method Requirements

Our method was running in MATLAB, so we required users to install MATLAB version on their operating systems.

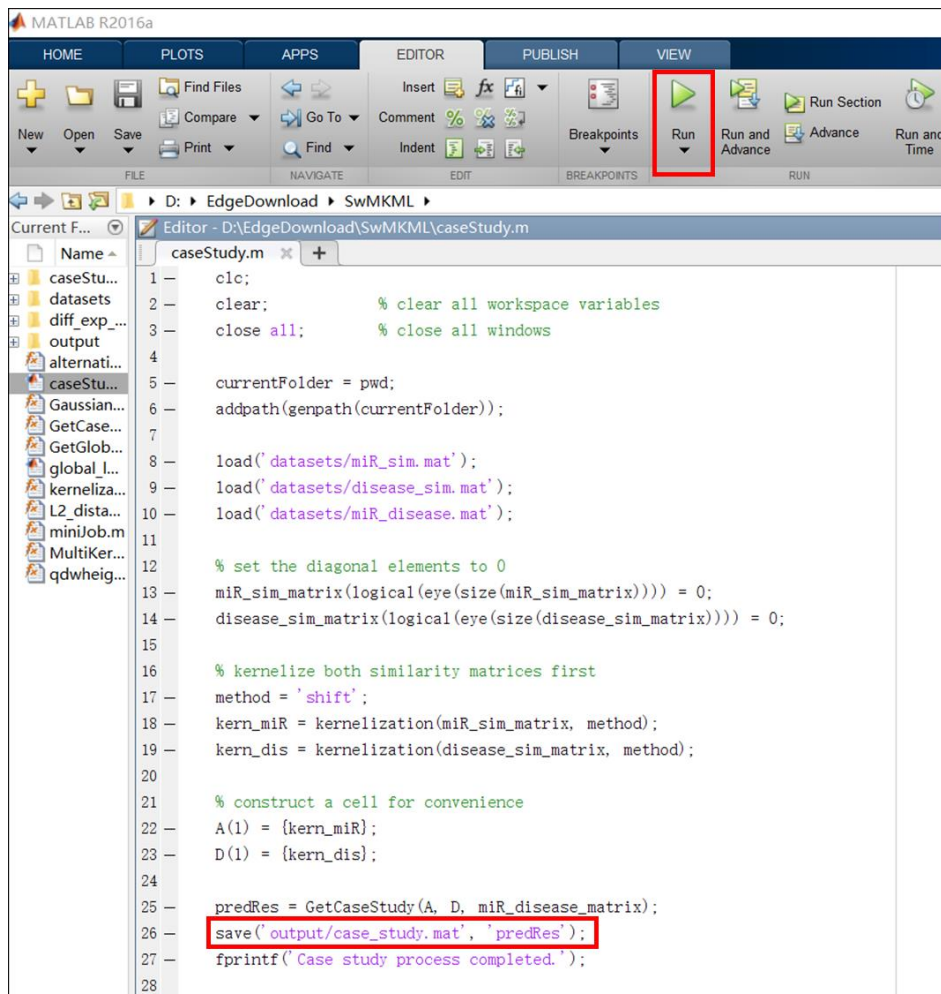
3. Usage

We provided two functions, case study and global leave-one-out cross-validation (LOOCV), for users. All the datasets used in the code, i.e. miRNA functional similarity, disease semantic similarity and miRNA-

disease associations are all provided in the corresponding '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	12	13	14	15	16	1
1	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	5.7521e...	0.9998 ...	3.7446e...	0.9997 ...	0.9997 ...	0.9997 ...	1.1852e...	3.6696e...	3.4680e...	2.8892e...	1.7414e...	-2.0 ^
2	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	5.4527e...	0.9998 ...	3.4664e...	0.9997 ...	1.0234e...	0.9997 ...	1.0982e...	3.4975e...	3.2106e...	2.6532e...	1.6302e...	-2.3
3	0.9997 ...	1.1293e...	0.9997 ...	0.9997 ...	0.9998 ...	5.4405e...	0.9998 ...	3.5451e...	0.9997 ...	1.0073e...	0.9997 ...	1.0645e...	3.4279e...	3.2239e...	2.6955e...	1.5823e...	-2.3
4	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	5.4703e...	0.9998 ...	3.9054e...	0.9997 ...	0.9997 ...	1.2729e...	1.2272e...	3.5437e...	3.2429e...	2.5657e...	1.7234e...	1.89
5	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	0.9997 ...	0.9998 ...	4.2157e...	0.9997 ...	0.9997 ...	1.2277e...	1.1676e...	3.4570e...	3.1227e...	2.6447e...	1.6277e...	8.02
6	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	4.8739e...	0.9998 ...	3.1280e...	0.9997 ...	0.9997 ...	1.3054e...	9.4356e...	3.0094e...	2.7621e...	2.1731e...	1.3363e...	-2.4
7	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	0.9997 ...	0.9998 ...	3.9017e...	0.9997 ...	9.4766e...	1.2937e...	1.0528e...	3.2518e...	3.0233e...	2.4632e...	1.4478e...	-1.8
8	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	4.7479e...	0.9998 ...	3.0240e...	0.9997 ...	8.6041e...	0.9997 ...	9.3558e...	2.8507e...	2.7098e...	2.1460e...	1.2987e...	-2.1
9	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	4.8421e...	0.9998 ...	3.0753e...	0.9997 ...	8.5562e...	0.9997 ...	9.8235e...	2.9829e...	2.7849e...	2.2117e...	1.3609e...	-1.7
10	0.9997 ...	9.3905e...	0.9997 ...	0.9997 ...	0.9998 ...	4.5904e...	0.9997 ...	3.0394e...	0.9997 ...	8.6742e...	0.9997 ...	7.5985e...	2.6321e...	2.4625e...	1.8373e...	1.0665e...	-1.9
11	0.9997 ...	9.5435e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9996 ...	0.9997 ...	3.7369e...	0.9997 ...	8.6326e...	1.2101e...	9.4058e...	3.1413e...	2.7670e...	2.1402e...	1.3230e...	-8.4
12	5.3433e...	9.3048e...	0.9997 ...	8.2715e...	0.9998 ...	0.9997 ...	0.9997 ...	4.2257e...	0.9997 ...	0.9997 ...	7.1212e...	3.0404e...	2.9553e...	2.1245e...	1.1993e...	-3.9	
13	0.9997 ...	9.6891e...	0.9997 ...	0.9997 ...	0.9998 ...	3.6783e...	0.9998 ...	2.5367e...	0.9997 ...	0.9997 ...	0.9997 ...	6.4217e...	2.6827e...	2.1239e...	1.8787e...	1.0623e...	1.87
14	4.3720e...	7.7489e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9996 ...	0.9997 ...	0.9996 ...	0.9997 ...	7.4716e...	0.9997 ...	5.9975e...	2.3779e...	2.0239e...	1.7435e...	9.8735e...	-1.0
15	4.8336e...	8.2574e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9996 ...	0.9997 ...	8.0515e...	0.9997 ...	6.2299e...	2.4411e...	2.0723e...	1.8280e...	1.0216e...	-6.9
16	0.9997 ...	9.2120e...	0.9997 ...	0.9997 ...	1.4031e...	3.6190e...	0.9997 ...	2.3675e...	0.9997 ...	0.9997 ...	0.9997 ...	7.8702e...	2.4188e...	2.0207e...	1.7827e...	9.9464e...	3.71
17	0.9997 ...	0.9997 ...	1.0607e...	0.9997 ...	0.9997 ...	4.3971e...	0.9997 ...	3.2290e...	7.5868e...	0.9997 ...	0.9997 ...	1.1832e...	3.3087e...	2.7926e...	2.5655e...	1.5841e...	4.36
18	0.9997 ...	0.9997 ...	0.9997 ...	7.5138e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9996 ...	0.9997 ...	0.9997 ...	0.9997 ...	7.3347e...	2.8526e...	2.2002e...	1.8898e...	1.1781e...	2.53
19	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9998 ...	3.9517e...	0.9998 ...	2.3672e...	0.9997 ...	9.6497e...	0.9997 ...	6.1451e...	2.6728e...	2.2910e...	1.6872e...	9.7733e...	3.79
20	0.9997 ...	0.9997 ...	0.9997 ...	9.4972e...	0.9998 ...	7.4094e...	0.9998 ...	0.9997 ...	8.8750e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	4.7528e...	5.40
21	6.7440e...	0.9997 ...	0.9997 ...	8.8539e...	0.9997 ...	7.0181e...	0.9997 ...	0.9997 ...	8.1036e...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9997 ...	0.9996 ...	5.93
22	4.6653e...	7.8432e...	8.8961e...	0.9997 ...	0.9997 ...	3.4649e...	0.9997 ...	2.6131e...	0.9997 ...	0.9997 ...	0.9997 ...	1.4613e...	2.7159e...	0.9996 ...	1.9951e...	1.6359e...	0.91 v

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:\ EdgeDownload \SwMKML', it is also the same under LINUX environment):

```
D:\EdgeDownload\SwMKML>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

Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 1
Predicting score is : 7.578959e-05
The current ranking is : 5.675000e+02

Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 2
Predicting score is : 7.277279e-05
The current ranking is : 664

Experiment type      : Global cross validation
Total steps are     : 6088
Current step is     : 3
Predicting score is : 7.100742e-05
The current ranking is : 738

```

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

globalPosition														
1x6088 double														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	567.5000	664	738	1.1045e...	1270	591.5000	678	692.5000	694.5000	873	875.5000	1372	1641	96
2														
3														

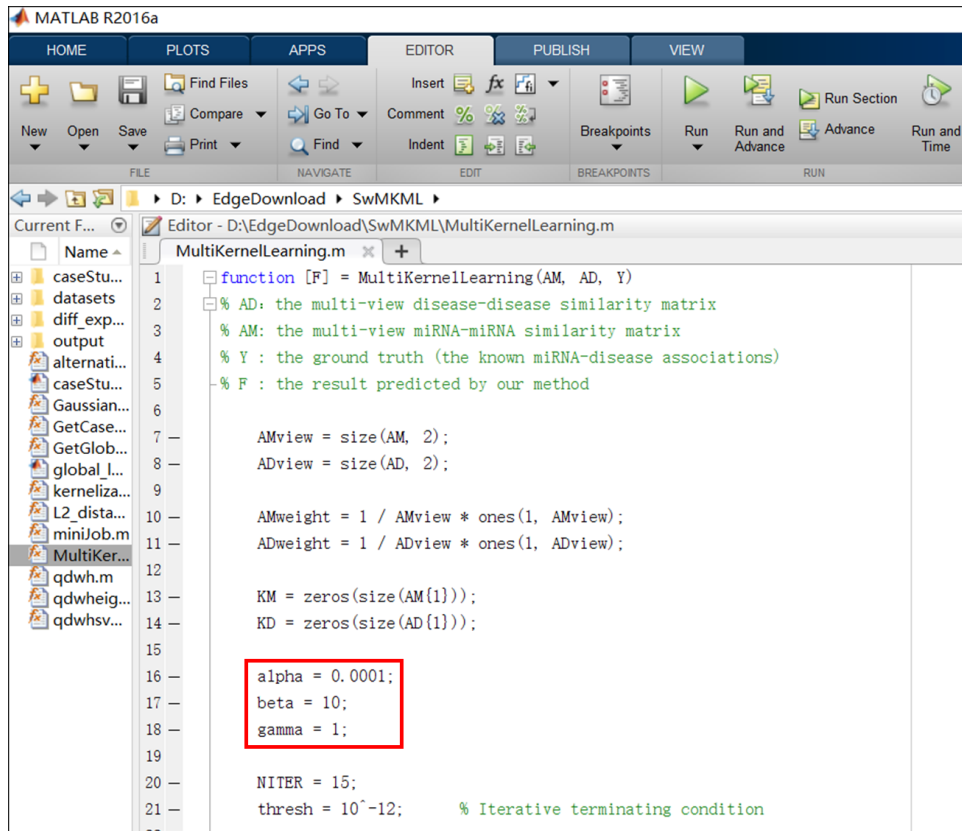
where each number, i.e. 567.5000, 664, 738 and etc., represent the average ranking of the known miRNA-disease association tested in turn.

The program can also be executed in standard command-line mode as follows:

```
D:\EdgeDownload\SwMKML>matlab -nodisplay -nodesktop -nosplash -r "global_loocv;exit;"
```

4. Parameters

There are three parameters alpha, beta and gamma in SwMKML. The default values for the three parameters are 1e-4, 10, 1, respectively. Users can change their value in "MultiKernelLearning.m" file.



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: wspzx9027@163.com.