Manual

MRMD3.0: a python tool and webserver for dimensionality reduction and data visualization through ensemble strategy

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Institutions

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GitHub: https://github.com/heshida01/MRMD3.0

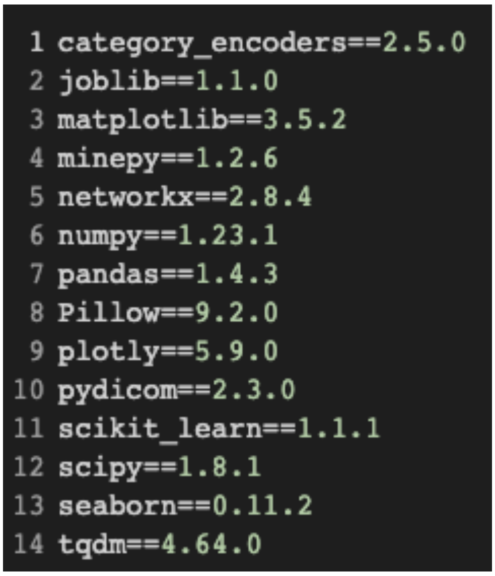
Webserver: http://lab.malab.cn/soft/MRMDv3/home.html

MRMD Version: 3.0

Content

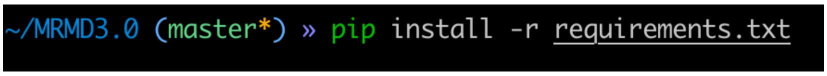
1. Installation

MRMD3.0 is an open-source Python-based toolkit, which operates depending on the Python environment (Python Version 3.0 or above). It can be run on multi-OS systems (such as Windows, Mac and Linux operating systems). Before running MRMD3.0, the user should make sure all the following packages are installed:



```
category_encoders==2.5.0
joblib==1.1.0
matplotlib==3.5.2
minepy==1.2.6
networkx==2.8.4
numpy==1.23.1
pandas==1.4.3
Pillow==9.2.0
plotly==5.9.0
pydicom==2.3.0
scikit_learn==1.1.1
scipy==1.8.1
seaborn==0.11.2
tqdm==4.64.0
```

A faster way to install them is you can install them in MRMD3.0 folder via command:



```
~/MRMD3.0 (master*) » pip install -r requirements.txt
```

2. feature rank and Ensemble methods overview

MRMD3.0 has many built-in feature rank methods, divided into three types: filtering, wrapper and embedded methods. The methods used for ranking feature and combine include PageRank, LeaderRank, HITS and LeaderRank.

2.1 feature rank

In the previous version of MRMD 2.0, we only used seven feature sorting algorithms. We have added 20 methods in the latest MRMD3.0. These methods are mainly from sickit-learn, minepy or our implementation. MRMD3.0 has also optimized the calculation speed, and we have strengthened the parallelism of the code. At the same time, in the experiment, we found that the original mRMR algorithm was too computationally complex. In MRMD3.0, we used a fast mRMR calculation method (https://github.com/smazzanti/mrmr), which is mainly explained here.

Table 1. feature rank and ensemble me

type	method	No. variant	Ensemble strategy
Filter	ANOVA	1. Analysis of variance (ANOVA)	
	Chis Square	2. Chis Square	
	Mutual information	3. Mutual Information (MI) 4. Normalized Mutual Information(NMI) 5. Maximal Information Coefficient (MIC)	PageRank
	MRMD1.0	6. MRMD- Euclidean distance 7. MRMD-Cos distance 8. MRMD-Tan Coefficient	LeaderRank
	mRMR	9. F-test correlation difference (FCD) 10. F-test correlation quotient (FCQ)	HITS
Warpper	Recursive feature elimination	11. LogisticRegression, 12. SVM 13. DecisionTreeClassifier	
Embedded	Tree feature importanc	14. DecisionTreeClassifier, 15. RandomForestClassifier, 16. GradientBoostingClassifier 17. ExtraTreesClassifier 18. Adaboost 19. LightGBMClassifier	TrustRank
	Linear model	20. Lasso 21. Ridge 22. Elasticnet	

2.2 Ensemble strategy

PageRank is an excellent ranking algorithm which is widely used in the ranking task of search engines. MRMD3.0 applies it to the "voting" task, combining the results of each feature ranking algorithm to calculate the feature importance. Besides, MRMD3.0 also has three classic algorithms(HITS, LeaderRank and TrustRank).

PageRank

There are many link relationships between web pages on the Internet. If you can fully use these structures, it can significantly improve the quality of web search. PageRank assumes that multiple web pages will point to a good web page and then calculates the PageRank value by the number of links and degrees of nodes.

HITS

HITS is an algorithm based on a keyword query. The algorithm requires query operations to obtain some web pages as the root set and then expand the web pages that have direct links to the web pages in the root set to the base set.

LeaderRank

The LeaderRank algorithm adds a global node to the original network graph, thereby improving the entire network's connectivity and ensuring the algorithm's convergence speed and robustness. We can also learn from this idea and add a global feature node connected to all features in the directed graph of features.

TrustRank

TrustRank requires human involvement to filter out high-quality torrent pages, but this does not apply and feature ranking because it is difficult for human methods to empirically determine whether a feature is important for a classification task. Therefore, the implementation method of this work is first to select the first few pages provided by PageRank as the features with high importance as seed features and then use this algorithm to rank the features.

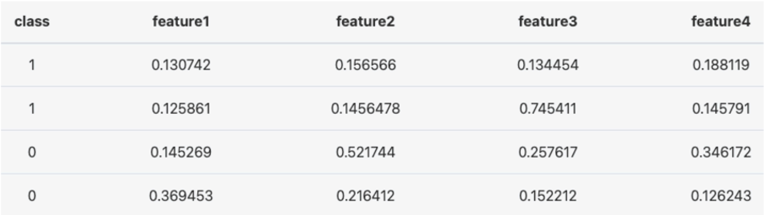
3 Input Format of MRMD3.0

MRMD3.0 requires the input of a **2d matrix** with labels, supports multi-label datasets, and belongs to supervised learning. The file format can be CSV, libSVM or Arff.

Tip: label must be placed in the first column in CSV and LibSVM.
The numeric type must be an integer.

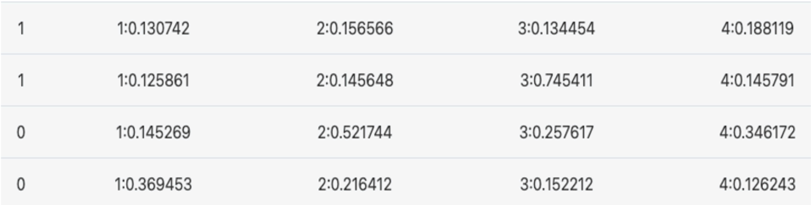
Example：

CSV



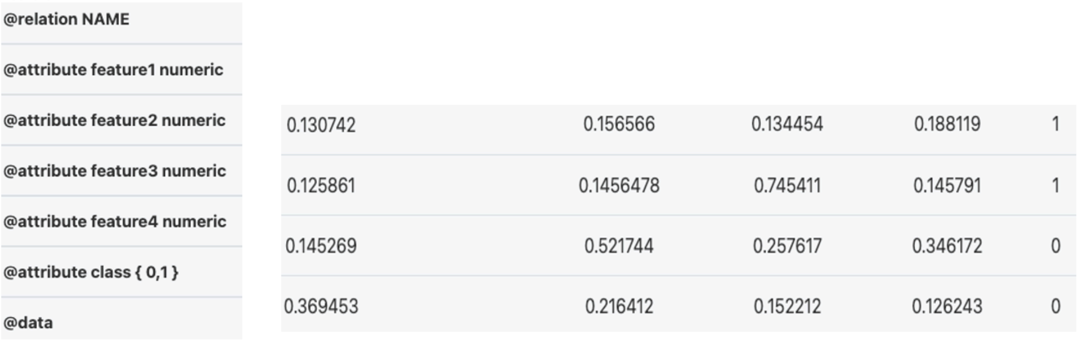
class	feature1	feature2	feature3	feature4
1	0.130742	0.156566	0.134454	0.188119
1	0.125861	0.1456478	0.745411	0.145791
0	0.145269	0.521744	0.257617	0.346172
0	0.369453	0.216412	0.152212	0.126243

libsvm



1	1:0.130742	2:0.156566	3:0.134454	4:0.188119
1	1:0.125861	2:0.145648	3:0.745411	4:0.145791
0	1:0.145269	2:0.521744	3:0.257617	4:0.346172
0	1:0.369453	2:0.216412	3:0.152212	4:0.126243

Arff



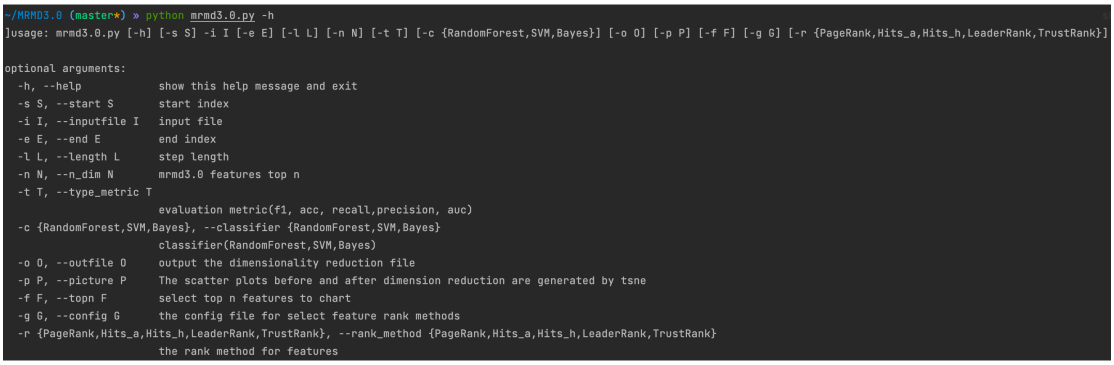
@relation NAME
@attribute feature1 numeric
@attribute feature2 numeric
@attribute feature3 numeric
@attribute feature4 numeric
@attribute class { 0,1 }
@data

0.130742	0.156566	0.134454	0.188119	1
0.125861	0.1456478	0.745411	0.145791	1
0.145269	0.521744	0.257617	0.346172	0
0.369453	0.216412	0.152212	0.126243	0

4 Command Version

MRMD3.0 provides many parameters for users to choose. You can usually get good results with the default parameters by giving the input and output files. Below we will introduce the critical parameters with specific examples.

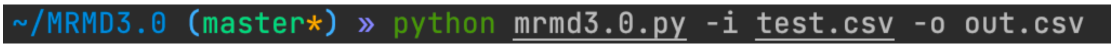
https://github.com/heshida01/MRMD3.0



```
~/MRMD3.0 (master*) » python mrmd3.0.py -h
]usage: mrmd3.0.py [-h] [-s S] -i I [-e E] [-l L] [-n N] [-t T] [-c {RandomForest,SVM,Bayes}] [-o O] [-p P] [-f F] [-g G] [-r {PageRank,Hits_a,Hits_h,LeaderRank,TrustRank}]

optional arguments:
  -h, --help            show this help message and exit
  -s S, --start S       start index
  -i I, --inputfile I   input file
  -e E, --end E         end index
  -l L, --length L      step length
  -n N, --n_dim N       mrmd3.0 features top n
  -t T, --type_metric T
                        evaluation metric(f1, acc, recall,precision, auc)
  -c {RandomForest,SVM,Bayes}, --classifier {RandomForest,SVM,Bayes}
                        classifier(RandomForest,SVM,Bayes)
  -o O, --outfile O     output the dimensionality reduction file
  -p P, --picture P     The scatter plots before and after dimension reduction are generated by tsne
  -f F, --topn F        select top n features to chart
  -g G, --config G      the config file for select feature rank methods
  -r {PageRank,Hits_a,Hits_h,LeaderRank,TrustRank}, --rank_method {PageRank,Hits_a,Hits_h,LeaderRank,TrustRank}
                        the rank method for features
```

Basic:



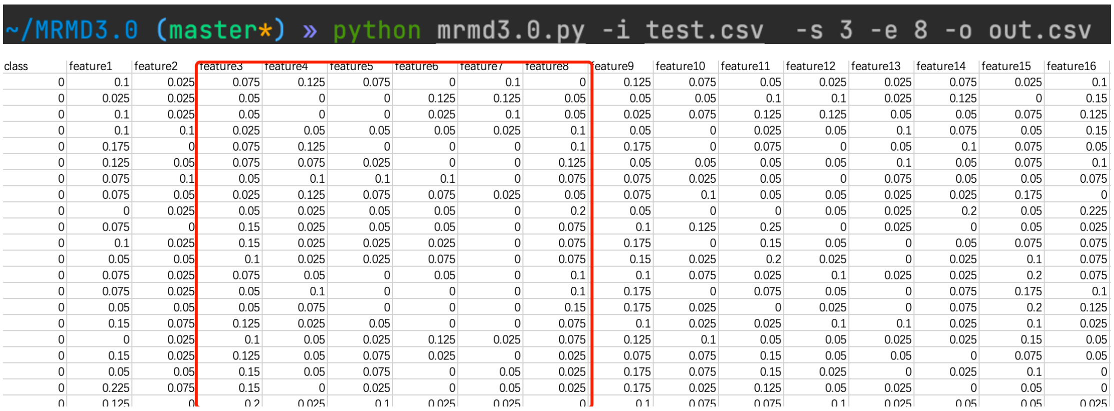
```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv -o out.csv
```

Customize:

1) Select an interval of data for dimensionality reduction

Parameters: -s start index ; -e end index;

Note: Under this parameter, MRMD3.0 will directly select and rank the top N features without performing feature search on the dataset. Usually, start_index(3) and end_index (8) are used together to reduce the dimensionality of a certain range(in this demo 8 - 3) of data features. By default, MRMD3.0 performs dimensionality reduction on all features (**start_index = 1 and end_index = -1)**

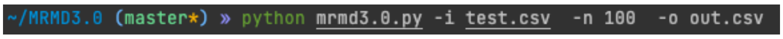


```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -s 3 -e 8 -o out.csv
```

class	feature1	feature2	feature3	feature4	feature5	feature6	feature7	feature8	feature9	feature10	feature11	feature12	feature13	feature14	feature15	feature16
0	0.1	0.025	0.075	0.125	0.075	0	0.1	0	0.125	0.075	0.05	0.025	0.025	0.075	0.025	0.1
0	0.025	0.025	0.05	0	0	0.125	0.125	0.05	0.05	0.05	0.1	0.1	0.025	0.125	0	0.15
0	0.1	0.025	0.05	0	0	0.025	0.1	0.05	0.025	0.075	0.125	0.125	0.05	0.05	0.075	0.125
0	0.1	0.1	0.025	0.05	0.05	0.05	0.025	0.1	0.05	0	0.025	0.05	0.1	0.075	0.05	0.15
0	0.175	0	0.075	0.125	0	0	0	0.1	0.175	0	0.075	0	0.05	0.1	0.075	0.05
0	0.125	0.05	0.075	0.075	0.025	0	0	0.125	0.05	0.05	0.05	0.05	0.1	0.05	0.075	0.1
0	0.075	0.1	0.05	0.1	0.1	0.1	0	0.075	0.075	0.025	0.05	0	0.075	0.05	0.05	0.075
0	0.075	0.05	0.025	0.125	0.075	0.075	0.025	0.05	0.075	0.1	0.05	0.05	0.025	0.025	0.175	0
0	0	0.025	0.05	0.025	0.05	0.05	0	0.2	0.05	0	0	0.05	0.025	0.2	0.05	0.225
0	0.075	0	0.15	0.025	0.05	0.05	0	0.075	0.1	0.125	0.25	0	0.025	0	0.05	0.025
0	0.1	0.025	0.15	0.025	0.025	0.025	0	0.075	0.175	0	0.15	0.05	0	0.05	0.075	0.075
0	0.05	0.05	0.1	0.025	0.025	0.075	0	0.075	0.15	0.025	0.2	0.025	0	0.025	0.1	0.075
0	0.075	0.025	0.075	0.05	0	0.05	0	0.1	0.1	0.075	0.025	0.1	0.025	0.025	0.2	0.075
0	0.075	0.025	0.05	0.1	0	0	0	0.1	0.175	0	0.075	0.05	0	0.075	0.175	0.1
0	0.05	0.05	0.05	0.075	0	0	0	0.15	0.175	0.025	0	0.025	0	0.075	0.2	0.125
0	0.15	0.075	0.125	0.025	0.05	0	0	0.075	0.1	0.025	0.025	0.1	0.1	0.025	0.1	0.025
0	0	0.025	0.1	0.05	0.025	0.125	0.025	0.075	0.125	0.1	0.05	0.05	0.025	0.025	0.15	0.05
0	0.15	0.025	0.125	0.05	0.075	0.025	0	0.025	0.075	0.075	0.15	0.05	0.05	0	0.075	0.05
0	0.05	0.05	0.15	0.05	0.075	0	0.05	0.025	0.175	0.075	0.15	0.025	0	0.025	0.1	0
0	0.225	0.075	0.15	0	0.025	0	0.05	0.025	0.175	0.025	0.125	0.05	0.025	0	0.05	0
0	0.125	0	0.2	0.025	0.1	0.025	0.025	0	0.1	0.075	0.075	0.1	0.025	0.05	0.05	0.025

2)Select the top n features

Parameters: -n 100
Default: None

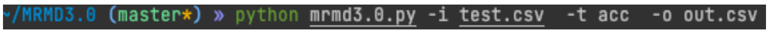


```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -n 100  -o out.csv
```

Note: which is automatically calculated by default and does not need to be set, on the contrary, you can also set it to 100, it will save the top 100 features.

3) Choose Evaluation Metrics

This parameter is the evaluation metric for cross-validation when using IFS.



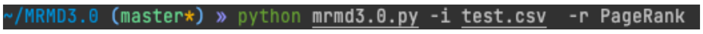
```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -t acc  -o out.csv
```

Parameters: -t f1 | acc | recall | precision | AUC
Default f1

Note: When using the IFS method to select the most suitable dimensions, the recommended metrics are as follows: for balanced data, accuracy is recommended; For slightly imbalanced data that require a balance between recall and precision, the F1 score is recommended; If your application requires minimizing false positives (incorrectly predicting positive cases), then you should focus on precision. If your application needs to minimize false negatives (failing to identify actual positive cases), then recall should be the primary focus. and for extremely imbalanced data, The AUC parameter is recommended.

4) Select an ensemble strategy for feature ranking

Parameters: -r PageRank | Hits_a | Hits_h | LeaderRank | TrustRank
Default:PageRank



```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -r PageRank
```

Note:
PageRank: Calculate the weight of a node based on the number of incoming links (and the weight of the link source) of each node. The advantage is that it is simple and easy to understand.

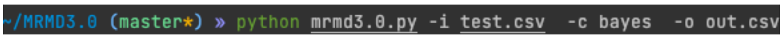
TrustRank: Some high-quality features are added before MRMD3.0 feature sorting, and these features need to be obtained in advance by other methods. MRMD3.0 uses some features recommended by PageRank by default.
HITS: The HITS algorithm takes into account both incoming and outgoing link characteristics. Which method to choose depends. Hubs focus on pages that are linked to by authoritative pages. authorities are pages with links from the hub.

LeaderRank: It not only considers incoming links (like Pagerank), but also outgoing links and local network structure. A key feature of Leaderrank is that it uses a global "ground node" interconnected with all other nodes to solve the problems of rank leakage and rank pooling. The advantage of LeaderRank is that it can better capture the local influence of nodes in the network.

5) Choose classifiers

This parameter is the classifier for cross-validation when using IFS.

Parameters: -c RandomForest | SVM | Bayes
default: RandomForest

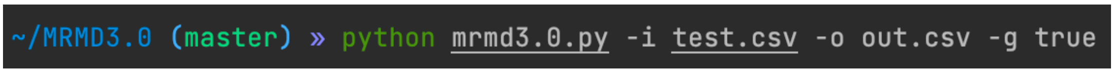


```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -c bayes  -o out.csv
```

Note: The classifier used when using IFS to select the most suitable dimension, choose according to your own needs, and recommend a random forest with stable performance.

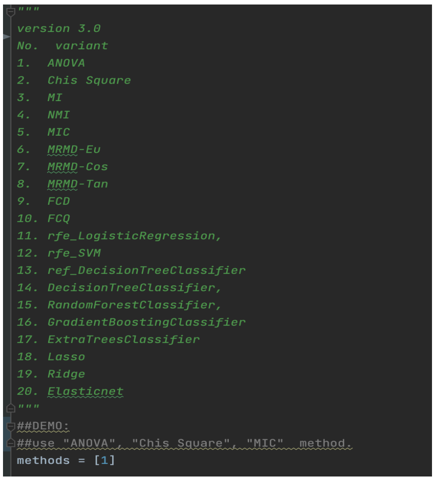
6) customize feature selection methods to rank feature

Parameters: -g True | False
Default: False



```
~/MRMD3.0 (master) » python mrmd3.0.py -i test.csv -o out.csv -g true
```

Note: If only one method is used, such as Lasso, MRMD3.0 only uses the Lasso method to rank the features and will no longer execute ensemble algorithms such as PageRank. Path: MRMD3.0/config.py

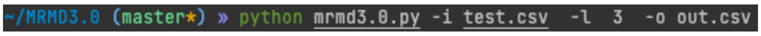


```
"""
version 3.0
No.  variant
1.   ANOVA
2.   Chis Square
3.   MI
4.   NMI
5.   MIC
6.   MRMD-Eu
7.   MRMD-Cos
8.   MRMD-Tan
9.   FCD
10.  FCQ
11.  rfe_LogisticRegression,
12.  rfe_SVM
13.  ref_DecisionTreeClassifier
14.  DecisionTreeClassifier,
15.  RandomForestClassifier,
16.  GradientBoostingClassifier
17.  ExtraTreesClassifier
18.  Lasso
19.  Ridge
20.  Elasticnet
"""
##DEMO:
##use "ANOVA", "Chis Square", "MIC"  method.
methods = [1]
```

7）Incremental feature selection step

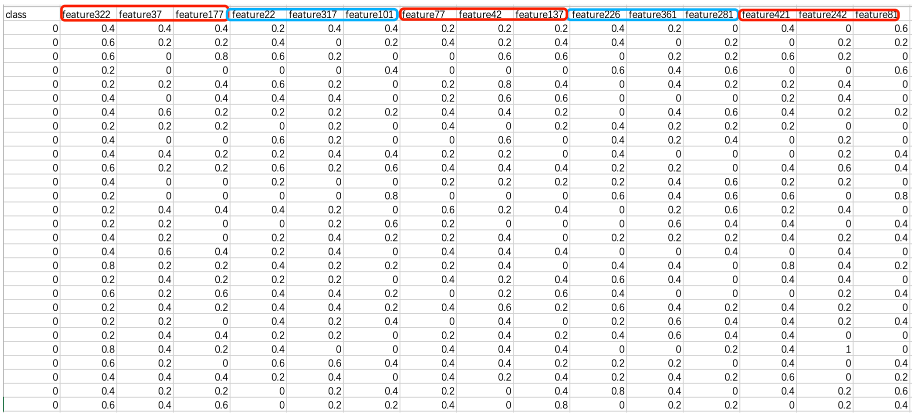
Parameters: -l step length
Default:1

Note: By default, when using the IFS feature search, each feature is added one by one to search. Here you can increase 1 to make the algorithm execute faster. For example, if it is changed to 3, every 3 features will be searched in groups.



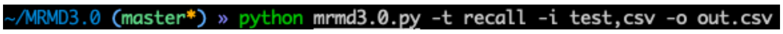
```
~/MRMD3.0 (master*) » python mrmd3.0.py -i test.csv  -l  3  -o out.csv
```

Note: By default, when using the IFS feature search, each feature is added one by one to search. Here you can increase 1 to make the algorithm execute faster. For example, if it is changed to 3, every 3 features will be searched in groups.



class	feature322	feature37	feature177	feature22	feature317	feature101	feature77	feature42	feature137	feature226	feature361	feature281	feature421	feature242	feature81
0	0.4	0.4	0.4	0.2	0.4	0.4	0.2	0.2	0.2	0.4	0.2	0	0.4	0	0.6
0	0.6	0.2	0.2	0.4	0	0.2	0.4	0.2	0.4	0.4	0	0.2	0	0.2	0.2
0	0.6	0	0.8	0.6	0.2	0	0	0.6	0.6	0	0.2	0.2	0.6	0.2	0
0	0.2	0	0	0	0	0.4	0	0	0	0.6	0.4	0.6	0	0	0.6
0	0.2	0.2	0.4	0.6	0.2	0	0.2	0.8	0.4	0	0.4	0.2	0.2	0.4	0
0	0.4	0	0.4	0.4	0.4	0	0.2	0.6	0.6	0	0	0	0.2	0.4	0
0	0.4	0.6	0.2	0.2	0.2	0.2	0.4	0.4	0.2	0	0.4	0.6	0.4	0.2	0.2
0	0.2	0.2	0.2	0	0.2	0	0.4	0	0.2	0.4	0.2	0.2	0.2	0	0
0	0.4	0	0	0.6	0.2	0	0	0.6	0	0.4	0.2	0.4	0	0.2	0
0	0.4	0.4	0.2	0.2	0.4	0.4	0.2	0.2	0	0.4	0	0	0	0.2	0.4
0	0.6	0.2	0.2	0.6	0.2	0.6	0.4	0.4	0.4	0.2	0.2	0	0.4	0.6	0.4
0	0.4	0	0	0.2	0	0	0.2	0.2	0.2	0.2	0.4	0.6	0.2	0.2	0
0	0.2	0	0	0	0	0.8	0	0	0	0.6	0.4	0.6	0.6	0	0.8
0	0.2	0.4	0.4	0.4	0.2	0	0.6	0.2	0.4	0	0.2	0.6	0.2	0.4	0
0	0.2	0.2	0	0	0.2	0.6	0.2	0	0	0	0.6	0.4	0.4	0	0.4
0	0.4	0.2	0	0.2	0.4	0.2	0.2	0.4	0	0.2	0.2	0.2	0.4	0.2	0.4
0	0.4	0.6	0.4	0.2	0.4	0	0.4	0.4	0.4	0	0	0.4	0	0.4	0
0	0.8	0.2	0.2	0.4	0.2	0.2	0.2	0.4	0	0.4	0.4	0	0.8	0.4	0.2
0	0.2	0.4	0.2	0.2	0.2	0	0.4	0.2	0.4	0.6	0.4	0	0.4	0.4	0
0	0.6	0.2	0.6	0.4	0.4	0.2	0	0.2	0.6	0.4	0	0	0	0.2	0.4
0	0.2	0.4	0.2	0.4	0.4	0.2	0.4	0.6	0.2	0.6	0.4	0.2	0.4	0.2	0
0	0.2	0.2	0	0.4	0.2	0.4	0	0.4	0	0.2	0.6	0.4	0.4	0.2	0.4
0	0.2	0.4	0.4	0.2	0.2	0	0.2	0.4	0.2	0.4	0.6	0.4	0.4	0	0
0	0.8	0.4	0.2	0.4	0	0	0.4	0.4	0.4	0	0	0.2	0.4	1	0
0	0.6	0.2	0	0.6	0.6	0.4	0.4	0.4	0.2	0.2	0.2	0	0.4	0	0.4
0	0.4	0.4	0.4	0.2	0.4	0	0.4	0.2	0.4	0.2	0.4	0.2	0.6	0	0.2
0	0.4	0.2	0.2	0	0.2	0.4	0.2	0	0.4	0.8	0.4	0	0.4	0.2	0.6
0	0.6	0.4	0.6	0	0.2	0.2	0.4	0	0.8	0	0.2	0.2	0	0.2	0.4

8) select evaluation metric for cross-validation
Parameters: -t   f1, acc, recall, precision, auc



```
~/MRMD3.0 (master*) » python mrmd3.0.py -t recall -i test,csv -o out.csv
```

$$\mathrm{acc} = \frac{\mathrm{TP} + \mathrm{TN}}{(\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN})}$$

$$\mathrm{precision} = \frac{\mathrm{TP}}{(\mathrm{TP} + \mathrm{FP})}$$

$$\mathrm{recall} = \frac{\mathrm{TP}}{(\mathrm{TP} + \mathrm{FN})}$$

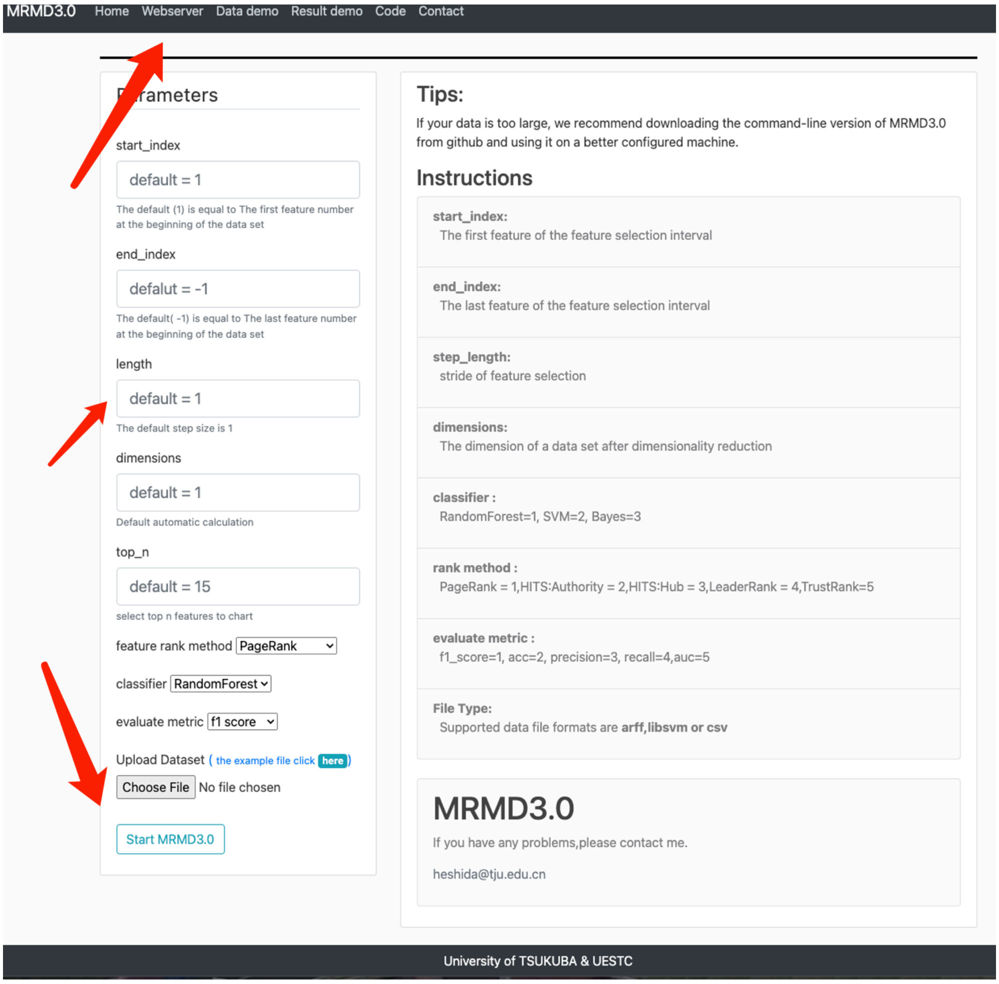
$$f1 = \frac{2 * \mathrm{precision} * \mathrm{recall}}{(\mathrm{precision} * \mathrm{recall})}$$

AUC (https://scikitlearn.org/stable/modules/generated/sklearn.metrics.auc.html)is the area under the receiver operating characteristic curve from prediction scores.

Note: When using the IFS method to select the most suitable dimensions, the recommended metrics are as follows: for balanced data, accuracy is recommended; For slightly imbalanced data that require a balance between recall and precision, the F1 score is recommended; If your application requires minimizing false positives (incorrectly predicting positive cases), then you should focus on precision. If your application needs to minimize false negatives (failing to identify actual positive cases), then recall should be the primary focus. and for extremely imbalanced data, The AUC parameter is recommended.

5 Online Webserver

The Webserver (**http://lab.malab.cn/soft/MRMDv3/home.html**) parameter usage is almost the same as the Standalone version. After opening the link, enter the corresponding parameters, upload the file, and wait for the result.



Parameters

start_index

default = 1

The default (1) is equal to The first feature number at the beginning of the data set

end_index

defalut = -1

The default(-1) is equal to The last feature number at the beginning of the data set

length

default = 1

The default step size is 1

dimensions

default = 1

Default automatic calculation

top_n

default = 15

select top n features to chart

feature rank method: PageRank

classifier: RandomForest

evaluate metric: f1 score

Upload Dataset (the example file click here)

Choose File No file chosen

Tips:

If your data is too large, we recommend downloading the command-line version of MRMD3.0 from github and using it on a better configured machine.

Instructions

start_index:
The first feature of the feature selection interval

end_index:
The last feature of the feature selection interval

step_length:
stride of feature selection

dimensions:
The dimension of a data set after dimensionality reduction

classifier :
RandomForest=1, SVM=2, Bayes=3

rank method :
PageRank = 1,HITS:Authority = 2,HITS:Hub = 3,LeaderRank = 4,TrustRank=5

evaluate metric :
f1_score=1, acc=2, precision=3, recall=4,auc=5

File Type:
Supported data file formats are **arff,libsvm or csv**

MRMD3.0

If you have any problems,please contact me.

heshida@tju.edu.cn

University of TSUKUBA & UESTC

After running, you will see the following page:
A: The highest metric of MRMD3.0 feature search post-cross-validation
B: Top N feature visualization chart C Score of features after ranking

Webserver Guide:
Parameters:

- **start_index**
  The start feature index of the feature selection (defalut 1)

- **end_index**
  The last feature index of the feature selection(defalut -1)

Note: Usually, start_index and end_index are used together to reduce the dimensionality of a certain range of data features. By default, MRMD3.0 performs dimensionality reduction on all features (**start_index = 1 and end_index = -1)**

- **length**
  stride of feature selection(defalut 1)

Note: By default, when using the IFS feature search, each feature is added one by one to search. Here you can increase 1 to make the algorithm execute faster. For example, if it is changed to 3, every 3 features will be searched in groups.

- **Top_n**
  Save top n features to chart

Note: default 15,include: violin plot, heatmap, stem map)

- **Dimensions**
  set the number of features for feature selection.

Note: which is automatically calculated by default and does not need to be set, on the contrary, you can also set it to k, it will save the top k features.

- **Classifier**
  Classifier to use when inferring the number of features via IFS
  （Randomforest,SVM,Bayes）

Note: The classifier used when using IFS to select the most suitable dimension, choose according to your own needs, and recommend a random forest with stable performance.

- **Rank method**
  Various ensemble strategies of MRMD3.0
  (PageRank ; HITS:Authority ;HITS:Hub ;LeaderRank ;TrustRank.)

Note:
PageRank: Calculate the weight of a node based on the number of incoming links (and the weight of the link source) of each node. The advantage is that it is simple and easy to understand.

TrustRank: Some high-quality features are added before MRMD3.0 feature sorting, and these features need to be obtained in advance by other methods. MRMD3.0 uses some features recommended by PageRank by default.

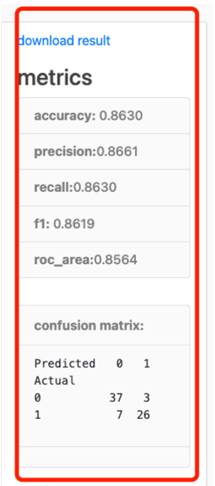
HITS: The HITS algorithm takes into account both incoming and outgoing link characteristics. Which method to choose depends. Hubs focus on pages that are linked to by authoritative pages. authorities are pages with links from the hub.

LeaderRank: It not only considers incoming links (like Pagerank), but also outgoing links and local network structure. A key feature of Leaderrank is that it uses a global "ground node" interconnected with all other nodes to solve the problems of rank leakage and rank pooling. The advantage of LeaderRank is that it can better capture the local influence of nodes in the network.

- **Evaluate metric**
  (f1_score, accuracy, precision, recall,auc)

Note: When using the IFS method to select the most suitable dimensions, the recommended metrics are as follows: for balanced data, accuracy is recommended; For slightly imbalanced data that require a balance between recall and precision, the F1 score is recommended; If your application requires minimizing false positives (incorrectly predicting positive cases), then you should focus on precision. If your application needs to minimize false negatives (failing to identify actual positive cases), then recall should be the primary focus. and for extremely imbalanced data, The AUC parameter is recommended.

Demo Result:



download result

metrics

accuracy: 0.8630

precision:0.8661

recall:0.8630

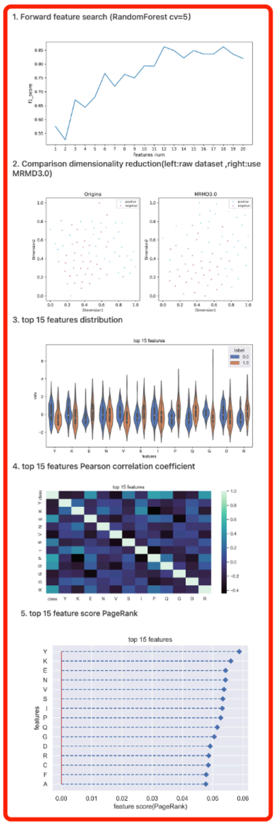
f1: 0.8619

roc_area:0.8564

confusion matrix:

```
Predicted   0   1
Actual
0          37   3
1           7  26
```

A



1. Forward feature search (RandomForest cv=5)

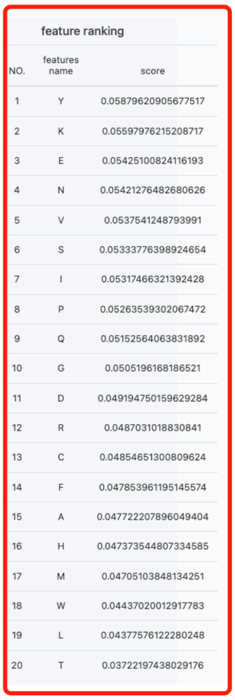
2. Comparison dimensionality reduction(left:raw dataset ,right:use MRMD3.0)

3. top 15 features distribution

4. top 15 features Pearson correlation coefficient

5. top 15 feature score PageRank

B



feature ranking

NO.	features name	score
1	Y	0.05879620905677517
2	K	0.05597976215208717
3	E	0.05425100824116193
4	N	0.05421276482680626
5	V	0.0537541248793991
6	S	0.05333776398924654
7	I	0.05317466321392428
8	P	0.05263539302067472
9	Q	0.05152564063831892
10	G	0.0505196168186521
11	D	0.049194750159629284
12	R	0.0487031018830841
13	C	0.04854651300809624
14	F	0.047853961195145574
15	A	0.047722207896049404
16	H	0.047373544807334585
17	M	0.04705103848134251
18	W	0.04437020012917783
19	L	0.04377576122280248
20	T	0.03722197438029176

C

6 Summary

MRMD3.0 is a comprehensive Python-based toolkit for dimensionality reduction. We provide 21 feature ranking algorithms and four ensemble strategies. In addition, MRMD3.0 uses the IFS feature search strategy to select features and automatically search for the size of the dimension after dimensionality reduction. In addition, compared with the previous version, an important change of MRMD3.0 is to support a single feature selection method, which is not available in the previous version. Finally, our MRMD3.0 can automatically draw five different types of charts to help users conduct data analysis.

Reference

Pedregosa, Fabian, et al. "Scikit-learn: Machine learning in Python." *the Journal of machine Learning research* 12 (2011): 2825-2830.

Ding, Chris, and Hanchuan Peng. "Minimum redundancy feature selection from microarray gene expression data." *Journal of bioinformatics and computational biology* 3.02 (2005): 185-205.

Zhao, Zhenyu, Radhika Anand, and Mallory Wang. "Maximum relevance and minimum redundancy feature selection methods for a marketing machine learning platform." *2019 IEEE international conference on data science and advanced analytics (DSAA)*. IEEE, 2019.

Albanese, Davide, et al. "Minerva and minepy: a C engine for the MINE suite and its R, Python and MATLAB wrappers." *Bioinformatics* 29.3 (2013): 407-408.

Zou, Quan, et al. "A novel features ranking metric with application to scalable visual and bioinformatics data classification." *Neurocomputing* 173 (2016): 346-354.

He, Shida., et al., MRMD2.0: A Python Tool for Machine Learning with Feature Ranking and Reduction. Current Bioinformatics, 2020. 15(10): p. 1213-1221.

Brin, Sergey, and Lawrence Page. "The anatomy of a large-scale hypertextual web search engine." *Computer networks and ISDN systems* 30.1-7 (1998): 107-117.

Kleinberg, Jon M. "Hubs, authorities, and communities." *ACM computing surveys (CSUR)* 31.4es (1999): 5-es.

Kleinberg, Jon M. "Authoritative sources in a hyperlinked environment." *Journal of the ACM (JACM)* 46.5 (1999): 604-632.

Lü, Linyuan, et al. "Leaders in social networks, the delicious case." *PloS one* 6.6 (2011): e21202.