12/15/2014

dl2

DL\_contact\_matrix\_load2-new10fold\_12\_15\_2014\_server.py

Python

settings = {}

settings['filename'] = 'ddi\_examples\_40\_60\_over2top\_diff\_name\_2014.txt'

settings['fisher\_mode'] = 'FisherM1'

settings['with\_auc\_score'] = False

settings['reduce\_ratio'] = 1

settings['SVM'] = 1

settings['DL'] = 0

settings['SAE\_SVM'] = 1

settings['SVM\_RBF'] = 1

settings['SAE\_SVM\_RBF'] = 1

settings['SVM\_POLY'] = 0

settings['DL\_S'] = 0

settings['DL\_U'] = 0

settings['finetune\_lr'] = 1

settings['batch\_size'] = 100

settings['pretraining\_interations'] = 5001

settings['pretrain\_lr'] = 0.001

settings['training\_epochs'] = 1502

settings['hidden\_layers\_sizes'] = [100, 100]

settings['corruption\_levels'] = [0,0]

dl3

DL\_contact\_matrix\_load2-new10fold\_12\_15\_2014\_server3.py

settings = {}

settings['filename'] = 'ddi\_examples\_40\_60\_over2top\_diff\_name\_2014.txt'

settings['fisher\_mode'] = 'FisherM1ONLY'

settings['with\_auc\_score'] = False

settings['reduce\_ratio'] = 1

settings['SVM'] = 1

settings['DL'] = 0

settings['SAE\_SVM'] = 1

settings['SVM\_RBF'] = 1

settings['SAE\_SVM\_RBF'] = 1

settings['SVM\_POLY'] = 0

settings['DL\_S'] = 0

settings['DL\_U'] = 0

settings['finetune\_lr'] = 1

settings['batch\_size'] = 100

settings['pretraining\_interations'] = 5003

settings['pretrain\_lr'] = 0.001

settings['training\_epochs'] = 1503

settings['hidden\_layers\_sizes'] = [100, 100]

settings['corruption\_levels'] = [0,0]

Before 10/29/2014 Every python script and every DDI tenfoldcross validation are in Fishermode FisherM1Only.

Need to rewrite the code of

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN

08/25/2014

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave40-75\_Examples\_2010\_real\_selected\_1to5.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

05/22

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave40-75\_Examples\_2010\_real\_selected.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

failed

05/21

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave40-75\_Examples\_2010\_real\_selected\_1to5.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-5-22 4:5 FINISHED.

Number of total DDI is: 5

Number of successed DDI is: 1

Number of total sequence is: 47

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.085%

The baseline recall: 69.067%

The baseline precision: 1.065%

Testing AUC: 87.638%

Testing recall: 70.851%

Testing precision: 0.912%

Testing f\_measure: 1.793%

Training accuracy: 99.420%

Training recall: 99.741%

Training precision: 99.115%

Training f\_measure: 99.424%

Maybe problems in the cross validation code.

05/20

run3DID\_CrossValidation\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_STAT\_75\_125\_examples\_201012MAY2014.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

05/13

dl8

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('list\_of\_SUCCESS\_log\_run3DID\_STAT\_75\_125\_examples\_201012MAY2014.txt')

ContactMapsOn3DID\_2010\_new('list\_of\_SUCCESS\_log\_run3DID\_STAT\_75\_125\_examples\_201012MAY2014.txt')

run3DID\_CrossValidation\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_STAT\_75\_125\_examples\_201012MAY2014.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/16

Sending a stop signal to all the labs ... stopped.

2014-5-15 11:56 FINISHED.

Number of total DDI is: 61

Number of successed DDI is: 38

Number of total sequence is: 3632

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 99.546%

The baseline recall: 97.733%

The baseline precision: 98.342%

Testing AUC: 99.499%

Testing recall: 98.624%

Testing precision: 98.304%

Testing f\_measure: 98.145%

Training accuracy: 99.985%

Training recall: 99.977%

Training precision: 99.993%

Training f\_measure: 99.985%

05/11

run3DID\_CrossValidation\_load\_DL\_remote('list\_DDI\_200\_500\_multiTop\_example\_real.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

2014-5-13 :15 FINISHED.

Number of total DDI is: 28

Number of successed DDI is: 23

Number of total sequence is: 5895

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 98.572%

The baseline recall: 96.806%

The baseline precision: 93.232%

Testing AUC: 98.637%

Testing recall: 97.184%

Testing precision: 93.218%

Testing f\_measure: 93.142%

Training accuracy: 99.643%

Training recall: 99.607%

Training precision: 99.682%

Training f\_measure: 99.639%

1/16

05/08

dl84

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_9\_16.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

dl83

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_1\_8.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

dl87

run3DID\_CrossValidation\_load\_DL\_remote('list\_DDI\_200\_500\_multiTop\_example\_real.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-5-10 1:9 FINISHED.

Number of total DDI is: 28

Number of successed DDI is: 23

Number of total sequence is: 5895

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 99.162%

The baseline recall: 97.629%

The baseline precision: 94.731%

Testing AUC: 99.199%

Testing recall: 97.784%

Testing precision: 94.793%

Testing f\_measure: 94.437%

Training accuracy: 99.434%

Training recall: 99.267%

Training precision: 99.601%

Training f\_measure: 99.428%

('current DDI:', 'RVT\_1\_int\_RVT\_thumb', 255)

AUC:

0.992607843137

0.988290196078

(2.9487665553046192, 0.0034877640292398184)

Recall:

0.970474509804

0.960168627451

(2.882348129216576, 0.0042849887380376388)

Precision:

0.993788235294

0.994125490196

(-0.29330850058815378, 0.76952585493886005)

('current DDI:', 'Transketolase\_C\_int\_Transket\_pyr', 231)

AUC:

0.948012987013

0.942398268398

(2.7294789333290068, 0.0068341061131281487)

Recall:

0.880047619048

0.854437229437

(4.4659097668979113, 1.2500268993531453e-05)

Precision:

0.888181818182

0.888125541126

(0.017275604351281618, 0.98623172419371952)

05/07

got 'list\_DDI\_200\_500\_example\_real.txt' But seem most same domain names or homodimer.

Dl87

ContactMapsOn3DID\_2010\_new('list\_DDI\_200\_500\_example\_real.txt')

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('list\_DDI\_200\_500\_multiTop\_example\_real.txt')

dl83

run3DID\_CrossValidation\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_STAT\_200\_275\_example\_1\_8.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

2014-5-8 3:1 FINISHED.

Number of total DDI is: 8

Number of successed DDI is: 5

Number of total sequence is: 1121

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 99.258%

The baseline recall: 98.255%

The baseline precision: 97.879%

Testing AUC: 99.400%

Testing recall: 98.227%

Testing precision: 97.941%

Testing f\_measure: 97.828%

Training accuracy: 99.844%

Training recall: 99.775%

Training precision: 99.914%

Training f\_measure: 99.844%

dl84

run3DID\_CrossValidation\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_STAT\_200\_275\_examples\_9\_16.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

05/04

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_1.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

198 examples

Sending a stop signal to all the labs ... stopped.

2014-5-6 17:39 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 198

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 96.789%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.194%

Testing recall: 94.176%

Testing precision: 91.941%

Testing f\_measure: 92.674%

Training accuracy: 92.923%

Training recall: 94.819%

Training precision: 91.378%

Training f\_measure: 93.044%

May2

Dl8

1/8

Lysine

dl8

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('list\_of\_SUCCESS\_log\_run3DID\_STAT\_200\_275\_example\_1\_8.txt')

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('list\_of\_SUCCESS\_log\_run3DID\_STAT\_200\_275\_example\_9\_16.txt')

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('list\_of\_SUCCESS\_log\_run3DID\_STAT\_200\_275\_example\_17\_22.txt')

run3DID\_STAT\_200\_250\_examples\_2010()

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_1.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-5-2 5:31 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 198

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 96.892%

The baseline recall: 92.247%

The baseline precision: 92.647%

Testing AUC: 97.734%

Testing recall: 93.675%

Testing precision: 94.021%

Testing f\_measure: 93.392%

Training accuracy: 98.837%

Training recall: 98.581%

Training precision: 99.088%

Training f\_measure: 98.831%

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_1.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2014-5-2 16:49 SUCCESS: Pico\_P1A\_int\_Rhv.

2014-5-2 16:49 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 198

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 98.166%

Testing recall: 97.845%

Testing precision: 92.489%

Testing f\_measure: 94.839%

Training accuracy: 94.986%

Training recall: 98.019%

Training precision: 92.414%

Training f\_measure: 95.134%

May 1st.

dl87

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished\_1.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

198 examples

Changed Ratio to 2:1 training validation ratio in split training set file.

run3DID\_CrossValidation\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

Apr 27

dl8

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-5-1 11:37 FINISHED.

Number of total DDI is: 4

Number of successed DDI is: 3

Number of total sequence is: 390

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 98.302%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 98.374%

Testing recall: 97.373%

Testing precision: 95.389%

Testing f\_measure: 96.178%

Training accuracy: 95.830%

Training recall: 96.629%

Training precision: 95.148%

Training f\_measure: 95.846%

dl84

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2014-4-28 17:28 FINISHED.

Number of total DDI is: 4

Number of successed DDI is: 3

Number of total sequence is: 390

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 98.454%

Testing recall: 98.900%

Testing precision: 95.170%

Testing f\_measure: 96.879%

Training accuracy: 97.058%

Training recall: 99.083%

Training precision: 95.309%

Training f\_measure: 97.139%

2014-4-27 22:55 ERROR: Lys\_int\_V-set. Message:

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished.txt', 'FisherM1', 'DLSTOP', 'DLSTOP', 1, 1)

April17 2014

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_finished.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

¼

2014-4-24 20:7 FINISHED.

Number of total DDI is: 4

Number of successed DDI is: 4

Number of total sequence is: 552

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 96.633%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.886%

Testing recall: 94.644%

Testing precision: 92.703%

Testing f\_measure: 93.170%

Training accuracy: 94.222%

Training recall: 94.851%

Training precision: 93.684%

Training f\_measure: 94.235%

Apr15 2014

dl82

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_unfinished\_1\_8.txt')

Apr27

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_unfinished\_1\_8.txt')

stopped.

dl85

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_unfinished\_9\_17.txt')

dl83

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_unfinished\_9\_17.txt')

2014-4-30 15:48 SUCCESS: RNA\_pol\_L\_int\_RNA\_pol\_Rpb1\_3

2014-5-2 7:18 SUCCESS: RNA\_pol\_Rpb1\_1\_int\_RNA\_pol\_Rpb2\_7

2014-4-30 15:48 SUCCESS: Ribosomal\_S4\_int\_S4

2014-5-2 3:43 SUCCESS: Transketolase\_C\_int\_Transket\_pyr

2014-4-30 15:48 SUCCESS: Ribosomal\_S5\_int\_Ribosomal\_S5\_C

2014-4-30 15:48 SUCCESS: Rieske\_int\_Ring\_hydroxyl\_A

2014-4-30 15:48 SUCCESS: RnaseH\_int\_RVT\_connect

2014-4-30 15:48 SUCCESS: RuBisCO\_large\_N\_int\_RuBisCO\_small

Apr8 2014

ContactMapsOn3DID\_2010\_new('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20.txt')

ContactMapsOn3DID\_2010\_new('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20\_first.txt')

dl8

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010\_equalPN('listOfDDIsHaveOver2InterfacesHave150-250Examples\_20.txt')

dl82

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'None', 'SVMLIGHT', 'LINEAR', 1, 1)

2014-4-11 16:51 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: None SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 95.745%

Testing recall: 94.546%

Testing precision: 88.105%

Testing f\_measure: 90.995%

Training accuracy: 91.528%

Training recall: 95.168%

Training precision: 88.710%

Training f\_measure: 91.825%

[du@ubuntu](mailto:du@ubuntu):~/Dropbox/Project/topologyTest$ du@ubuntu:~$ python GetDDIs\_150\_250Examples\_WithDifferentDomainNames.py

Get listOfDDIsHaveOver2InterfacesHave150-250Examples.txt

Remove some DDIs that has similar domains to 20.

listOfDDIsHaveOver2InterfacesHave150-250Examples\_20.txt

April 1 2011

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2014-4-5 :33 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.253%

Testing recall: 97.060%

Testing precision: 91.570%

Testing f\_measure: 94.124%

Training accuracy: 94.919%

Training recall: 97.859%

Training precision: 92.426%

Training f\_measure: 95.065%

2014-4-6 22:42 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.353%

Testing recall: 97.042%

Testing precision: 91.679%

Testing f\_measure: 94.172%

Training accuracy: 94.913%

Training recall: 97.858%

Training precision: 92.416%

Training f\_measure: 95.059%

March24

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'FIX\_RE', 'FIX\_RE', 1, 1)

½

error.

March20

dl8

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

½

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 100000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

2014-3-23 17:40 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 96.733%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.746%

Testing recall: 95.177%

Testing precision: 92.944%

Testing f\_measure: 93.891%

Training accuracy: 95.028%

Training recall: 96.113%

Training precision: 94.072%

Training f\_measure: 95.078%

%setup parameters

March 13

Dl84

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', ‘SAESVM’, ‘SAESVM’, 1, 1)

March17

dl8

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

¼

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 96.697%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.762%

Testing recall: 95.900%

Testing precision: 93.283%

Testing f\_measure: 94.341%

Training accuracy: 95.195%

Training recall: 96.941%

Training precision: 93.673%

Training f\_measure: 95.276%

Dl82

DLSTOP

dl82

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

incomplete

March 6

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1', 'DLSTOP', 'DLSTOP', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 500000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

2014-3-27 5:37 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1 SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 99.146%

Testing recall: 97.976%

Testing precision: 97.205%

Testing f\_measure: 97.283%

Training accuracy: 98.915%

Training recall: 99.233%

Training precision: 98.607%

Training f\_measure: 98.919%

March5

1/8

2014-3-8 :9 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 95.813%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.964%

Testing recall: 94.475%

Testing precision: 91.887%

Testing f\_measure: 92.759%

Training accuracy: 93.927%

Training recall: 95.869%

Training precision: 92.296%

Training f\_measure: 94.038%

Feb28

dl8

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-3-3 1:24 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 225

FisherMode: FisherM1ONLY SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 86.086%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 82.780%

Testing recall: 71.004%

Testing precision: 70.660%

Testing f\_measure: 69.223%

Training accuracy: 74.771%

Training recall: 72.663%

Training precision: 73.674%

Training f\_measure: 71.669%

Fail, because of parameters explosion.

Feb24

[du@ubuntu](mailto:du@ubuntu):~/Dropbox/Project/topologyTest$ python GetDDIsHaveOver2InterfacesHave200\_250Examples.py

number of lines wrote in listOfDDIsHaveOver2InterfacesHave200-250Examples.txt:31

ContactMapsOn3DID\_2010\_new('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt')

ddi Transketolase\_C\_int\_Transket\_pyr: success!

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_2010('listOfDDIsHaveOver2InterfacesHave200-250Examples\_first.txt')

done.

Feb12

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

½

Jan29

Dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

2014-2-3 2:2 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 94.003%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 93.784%

Testing recall: 85.445%

Testing precision: 88.363%

Testing f\_measure: 85.449%

Training accuracy: 88.619%

Training recall: 86.589%

Training precision: 89.457%

Training f\_measure: 87.283%

Dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

Jan21

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

½

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 100000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

FisherMode: FisherM1ONLY SVMMode: DL\_RE\_US Kernel: DL\_RE\_US, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 95.548%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 95.671%

Testing recall: 90.874%

Testing precision: 90.531%

Testing f\_measure: 89.870%

Training accuracy: 91.774%

Training recall: 92.191%

Training precision: 91.416%

Training f\_measure: 91.453%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL\_RE\_US', 1, 1)

1/8

Jan17

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1', 'DBN\_STOP', 'DBN\_STOP', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 100000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

alpha = 0.1; %default is 0.1

momentum = 0.5 %default is 0

plot = 0; % enable plotting

Jan16

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1', 'DBN\_STOP', 'DBN\_STOP', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 100000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

2014-1-16 15:13 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: DBN\_STOP Kernel: DBN\_STOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 70.561%

Testing recall: 55.211%

Testing precision: 57.392%

Testing f\_measure: 51.159%

Training accuracy: 65.394%

Training recall: 55.370%

Training precision: 63.115%

Training f\_measure: 52.750%

reconstruction error is big 108.

Dec29

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1', 'DLSTOP', 'DLSTOP', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 500000); %32 is default minibatchsize

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 98.181%

Testing recall: 96.523%

Testing precision: 94.220%

Testing f\_measure: 95.039%

Training accuracy: 98.752%

Training recall: 99.185%

Training precision: 98.343%

Training f\_measure: 98.759%

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DLSTOP', 'DLSTOP', 1, 1)

2013-12-31 19:30 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.419%

Testing recall: 93.921%

Testing precision: 91.398%

Testing f\_measure: 92.215%

Training accuracy: 94.732%

Training recall: 95.646%

Training precision: 94.041%

Training f\_measure: 94.780%

Dec28

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DLSTOP', 'DLSTOP', 1, 1)

2013-12-28 18:37 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.355%

Testing recall: 90.741%

Testing precision: 90.070%

Testing f\_measure: 89.662%

Training accuracy: 91.611%

Training recall: 91.548%

Training precision: 91.653%

Training f\_measure: 91.303%

dl83

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1ONLY', 'DLSTOP', 'DLSTOP', 1, 1)

2013-12-28 21:36 FINISHED.

Number of total DDI is: 3

Number of successed DDI is: 3

Number of total sequence is: 131

FisherMode: FisherM1ONLY SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 93.932%

Testing recall: 81.071%

Testing precision: 87.566%

Testing f\_measure: 81.907%

Training accuracy: 87.182%

Training recall: 83.498%

Training precision: 89.942%

Training f\_measure: 85.718%

Dec 27.

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_All

VectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLSTOP', 'DLSTOP', 1, 1)

[batchsize, numepochs]=setBatchsizeAndEpochs(size(train\_x, 1), 32, 100000); %32 is default minibatchsize

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0; %default is 0

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.181%

Testing recall: 77.391%

Testing precision: 81.356%

Testing f\_measure: 76.952%

Training accuracy: 86.324%

Training recall: 84.669%

Training precision: 86.556%

Training f\_measure: 84.403%

dl84

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1', 'DLSTOP', 'DLSTOP', 1, 1)

2013-12-29 2:53 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.732%

Testing recall: 96.640%

Testing precision: 93.708%

Testing f\_measure: 94.761%

Training accuracy: 97.568%

Training recall: 98.718%

Training precision: 96.539%

Training f\_measure: 97.606%

Dec26

dl82

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1', 'DLSTOP', 'DLSTOP', 1, 1)

FisherMode: FisherM1 SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.109%

Testing recall: 92.881%

Testing precision: 91.665%

Testing f\_measure: 91.527%

Training accuracy: 96.756%

Training recall: 97.572%

Training precision: 96.016%

Training f\_measure: 96.785%

dl84

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1ONLY', 'DLSTOP', 'DLSTOP', 1, 1)

2013-12-26 4:47 FINISHED.

Number of total DDI is: 3

Number of successed DDI is: 3

Number of total sequence is: 131

FisherMode: FisherM1ONLY SVMMode: DLSTOP Kernel: DLSTOP, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 93.931%

Testing recall: 80.994%

Testing precision: 86.803%

Testing f\_measure: 81.858%

Training accuracy: 87.214%

Training recall: 83.518%

Training precision: 89.985%

Training f\_measure: 85.762%

Dec20

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1', 'DL\_RE\_US', 'DL', 1, 1)

1/20

2013-12-22 21:21 FINISHED.

Number of total DDI is: 3

Number of successed DDI is: 3

Number of total sequence is: 131

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 86.034%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.956%

Testing recall: 69.861%

Testing precision: 77.941%

Testing f\_measure: 70.055%

Training accuracy: 76.093%

Training recall: 66.129%

Training precision: 83.430%

Training f\_measure: 72.017%

Dec17

dl82

run3DID\_Seq\_Par\_ChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1', 'DL\_RE\_US', 'DL', 1, 1)

Number of total DDI is: 3

Number of successed DDI is: 3

Number of total sequence is: 92

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 90.179%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.030%

Testing recall: 75.745%

Testing precision: 85.961%

Testing f\_measure: 78.488%

Training accuracy: 82.504%

Training recall: 74.447%

Training precision: 87.853%

Training f\_measure: 79.682%

Dec16

dl84

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL\_CLUSTER\_US', 'SAE\_US\_SVM', 1, 1)

%setup parameters

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

2013-12-18 14:43 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL\_CLUSTER\_US Kernel: SAE\_US\_SVM, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 90.209%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.209%

Testing recall: 54.187%

Testing precision: 71.925%

Testing f\_measure: 58.176%

Training accuracy: 75.267%

Training recall: 56.813%

Training precision: 92.087%

Training f\_measure: 64.179%

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1', 'DL\_RE\_US', 'DL', 1, 1)

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_multipleTopology150\_3.txt', 'FisherM1ONLY', 'DLSTOP', 'DL', 1, 1) Has error

Dec 10

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DLSTOP', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

%batchsize=size(train\_x, 1);

batchsize=32;

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

Change patient 30000 times. And evaluation every 10 runs.

Failled DLSTOP error.

%setup parameters

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=50000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

Dec5

2013-12-14 6:33 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: DL\_RE\_US Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 87.535%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.433%

Testing recall: 70.415%

Testing precision: 82.449%

Testing f\_measure: 72.780%

Training accuracy: 79.064%

Training recall: 71.127%

Training precision: 84.831%

Training f\_measure: 76.007%

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=50000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

Sending a stop signal to all the labs ... stopped.

2013-12-14 15:15 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL\_CLUSTER\_US Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

**The baseline AUC: 83.781%**

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 82.117%

Testing recall: 70.978%

Testing precision: 77.977%

Testing f\_measure: 72.682%

Training accuracy: 52.456%

Training recall: 86.430%

Training precision: 51.692%

Training f\_measure: 64.249%

This is not accurate because I changed the number of iterations. This using all examples for unsupervised is a little bit worse than using it only. This may be the unsupervised learned a generalized the manifold but training using limited examples exhaustly break the pretraining pattern and restrict to local examples again. And the number of examples is not statistically enough.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1ONLY', 'DL\_RE\_US', 'DL', 1, 1)

20

2013-12-9 11:56 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: DL\_RE\_US Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 93.359%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 93.026%

Testing recall: 80.641%

Testing precision: 87.654%

Testing f\_measure: 82.306%

Training accuracy: 85.894%

Training recall: 82.294%

Training precision: 88.961%

Training f\_measure: 84.632%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt', 'FisherM1', 'DL\_RE\_US', 'DL', 1, 1)

20

Dec4

run3DID\_CellectVectors\_Fishers\_aaIndex\_All\_Dec3('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt')

Dec3

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLSTOP', 'DL', 1, 1)

patient =3000

AUC 80% stop early.

Change patient to n+40000

Testing AUC: 83.352%

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DLSTOP', 'DL', 1, 1)

patient =3000

Testing AUC: 84.693%

need further improvement.

Nov23

dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'None', 'DL', 'DL', 1, 1)

2013-11-22 18:3 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: None SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 49.542%

Testing recall: 45.768%

Testing precision: 24.219%

Testing f\_measure: 31.079%

Training accuracy: 50.069%

Training recall: 47.518%

Training precision: 37.490%

Training f\_measure: 32.340%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'None', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-23 19:42 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: None SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 55.267%

Testing recall: 50.923%

Testing precision: 54.888%

Testing f\_measure: 51.591%

Training accuracy: 65.504%

Training recall: 66.688%

Training precision: 65.146%

Training f\_measure: 65.907%

Nov20

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SAESVM', 'L2', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=30000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

nonSparsityPenalty=0; %default is 3

dropoutFraction=0;

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=50000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

nonSparsityPenalty=0; %default is 3

dropoutFraction=0;

Testing AUC: 90.396%

numberOFFeature=size(train\_x, 2);

hiddenUnits=10;

batchsize=size(train\_x, 1);

numepochs=50000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

nonSparsityPenalty=0; %default is 3

dropoutFraction=0;

Testing AUC: 90.411%

Hidden units =5

Testing AUC: 89.907%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

2013-11-19 20:2 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.531%

Testing recall: 61.626%

Testing precision: 80.751%

Testing f\_measure: 64.546%

Training accuracy: 87.919%

Training recall: 87.801%

Training precision: 88.063%

Training f\_measure: 87.895%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'None', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-20 21:10 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: None SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 52.746%

Testing recall: 43.261%

Testing precision: 51.527%

Testing f\_measure: 45.482%

Training accuracy: 65.504%

Training recall: 66.688%

Training precision: 65.146%

Training f\_measure: 65.907%

Rerun.

FisherMode: None SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 53.309%

Testing recall: 43.261%

Testing precision: 51.697%

Testing f\_measure: 45.530%

Training accuracy: 65.504%

Training recall: 66.688%

Training precision: 65.146%

Training f\_measure: 65.907%

dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'None', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0; %default is 0

2 hidden layers.

Nov182013-11-21 1:31 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: None SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 55.455%

Testing recall: 35.405%

Testing precision: 53.802%

Testing f\_measure: 40.811%

Training accuracy: 84.890%

Training recall: 84.590%

Training precision: 85.203%

Training f\_measure: 84.835%

4 hidden

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SAESVM', 'L1', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

nonSparsityPenalty=0; %default is 3

AUC89.9

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

nonSparsityPenalty=0; %default is 3

AUC 90.5

Nov 17

Sending a stop signal to all the labs ... stopped.

2013-11-29 7:5 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.885%

Testing recall: 96.008%

Testing precision: 93.675%

Testing f\_measure: 94.209%

Training accuracy: 97.598%

Training recall: 98.746%

Training precision: 96.579%

Training f\_measure: 97.639%

Sending a stop signal to all the labs ... stopped.

2013-11-29 8:9 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.392%

Testing recall: 89.405%

Testing precision: 91.795%

Testing f\_measure: 89.613%

Training accuracy: 90.719%

Training recall: 89.877%

Training precision: 91.218%

Training f\_measure: 90.122%

Nov 15

dl84

2013-11-15 2:45 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 95.525%

Testing recall: 91.829%

Testing precision: 89.929%

Testing f\_measure: 90.117%

Training accuracy: 92.513%

Training recall: 93.905%

Training precision: 91.451%

Training f\_measure: 92.524%

2013-11-15 10:58 FINISHED.

Number of total DDI is: 14

Number of successed DDI is: 14

Number of total sequence is: 472

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.689%

Testing recall: 95.305%

Testing precision: 93.239%

Testing f\_measure: 93.519%

Training accuracy: 96.436%

Training recall: 97.979%

Training precision: 95.109%

Training f\_measure: 96.506%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 91.802%

Testing recall: 63.245%

Testing precision: 75.367%

Testing f\_measure: 64.275%

Training accuracy: 78.490%

Training recall: 76.538%

Training precision: 79.650%

Training f\_measure: 78.061%

Nov 13

Dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-13 14:9 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.120%

Testing recall: 95.522%

Testing precision: 89.792%

Testing f\_measure: 91.989%

Training accuracy: 92.810%

Training recall: 96.345%

Training precision: 90.721%

Training f\_measure: 93.122%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-13 20:59 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 98.537%

Testing recall: 97.627%

Testing precision: 93.433%

Testing f\_measure: 95.192%

Training accuracy: 97.321%

Training recall: 98.919%

Training precision: 95.983%

Training f\_measure: 97.405%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt’, 'FisherM1AAONLY', 'DL', 'DL', 1, 1)

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1AA1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-13 17:52 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: FisherM1AA1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.881%

Testing recall: 96.848%

Testing precision: 91.269%

Testing f\_measure: 93.696%

Training accuracy: 94.651%

Training recall: 97.684%

Training precision: 92.478%

Training f\_measure: 94.930%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_log\_run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep2531OCT2013.txt’, 'FisherM1AAONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

Nov12

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

2013-11-13 15:2 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 95.092%

Testing recall: 94.114%

Testing precision: 89.488%

Testing f\_measure: 91.045%

Training accuracy: 91.852%

Training recall: 94.693%

Training precision: 90.206%

Training f\_measure: 92.014%

dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

Nov11

Dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot=0;

2013-11-11 22:41 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 86.228%

Testing recall: 68.494%

Testing precision: 82.659%

Testing f\_measure: 72.285%

Training accuracy: 99.146%

Training recall: 99.344%

Training precision: 98.973%

Training f\_measure: 99.154%

local

%4 layer 1 1/2 1/4 1/8

numberOFFeature=size(train\_x, 2);

hiddenUnits=40;

batchsize=32;

numepochs=8000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.2; %default is 0

local

1 1 /2 /2

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=32;

numepochs=6000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

dl3

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-11 3:25 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.257%

Testing recall: 70.817%

Testing precision: 86.232%

Testing f\_measure: 72.896%

Training accuracy: 81.546%

Training recall: 80.321%

Training precision: 82.342%

Training f\_measure: 81.316%

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA3', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-12 4:2 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 115

Number of total sequence is: 115

FisherMode: FisherM1AA3 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.721%

Testing recall: 78.921%

Testing precision: 85.035%

Testing f\_measure: 78.782%

Training accuracy: 80.995%

Training recall: 83.634%

Training precision: 79.441%

Training f\_measure: 81.484%

Nov10

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

½

Testing AUC: 90.233%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=32;

numepochs=4000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.2; %default is 0

2013-11-11 :12 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 71.488%

Testing recall: 66.452%

Testing precision: 33.226%

Testing f\_measure: 44.301%

Training accuracy: 50.000%

Training recall: 66.667%

Training precision: 33.333%

Training f\_measure: 44.444%

Dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 0)

½

Testing AUC: 89.281%

Testing recall: 61.974%

Testing precision: 4.248%

Testing f\_measure: 7.134%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=32;

numepochs=4000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.2; %default is 0

2013-11-11 8:12 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 61.772%

Testing recall: 37.626%

Testing precision: 36.960%

Testing f\_measure: 32.728%

Training accuracy: 59.933%

Training recall: 47.689%

Training precision: 37.001%

Training f\_measure: 40.388%

Dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

1/2

2013-11-10 7:1 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.206%

Testing recall: 61.911%

Testing precision: 80.270%

Testing f\_measure: 66.135%

Training accuracy: 82.062%

Training recall: 71.898%

Training precision: 90.211%

Training f\_measure: 78.073%

Nov8

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

¼

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

1/2

2013-11-8 23:30 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.206%

Testing recall: 61.911%

Testing precision: 80.270%

Testing f\_measure: 66.135%

Training accuracy: 82.062%

Training recall: 71.898%

Training precision: 90.211%

Training f\_measure: 78.073%

Nov7

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

1/8

2013-11-7 20:45 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 86.831%

Testing recall: 59.676%

Testing precision: 82.531%

Testing f\_measure: 65.076%

Training accuracy: 80.493%

Training recall: 69.639%

Training precision: 89.115%

Training f\_measure: 76.138%

local

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=32;

numepochs=4000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.2; %default is 0

2013-11-11 11:52 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.293%

Testing recall: 60.411%

Testing precision: 79.979%

Testing f\_measure: 63.581%

Training accuracy: 92.561%

Training recall: 92.035%

Training precision: 93.020%

Training f\_measure: 92.521%

Nov6 run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

local

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=10000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

2013-11-11 10:49 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 82.021%

Testing recall: 59.969%

Testing precision: 80.090%

Testing f\_measure: 63.935%

Training accuracy: 97.870%

Training recall: 98.062%

Training precision: 97.687%

Training f\_measure: 97.874%

local

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=32;

numepochs=5000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

almost same as the above.

Nov5

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

2013-11-5 15:56 ERROR: PF00393.11\_int\_PF00393.11. Message: Undefined function or variable 'preTrain\_x'.

redo.

1/8

Error froget to give plot redo on Nov7

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

2013-11-7 18:30 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.535%

Testing recall: 55.336%

Testing precision: 78.832%

Testing f\_measure: 61.874%

Training accuracy: 87.962%

Training recall: 81.087%

Training precision: 94.173%

Training f\_measure: 85.865%

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

¼

2013-11-5 20:34 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 87.476%

Testing recall: 60.226%

Testing precision: 81.419%

Testing f\_measure: 65.102%

Training accuracy: 81.352%

Training recall: 71.122%

Training precision: 89.423%

Training f\_measure: 77.370%

dl83

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-11-5 19:53 ERROR: PF00712.11\_int\_PF02768.7. Message: Index exceeds matrix dimensions.

redo

Nov 4

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

1/32

2013-11-4 14:38 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.361%

Testing recall: 55.235%

Testing precision: 71.698%

Testing f\_measure: 57.664%

Training accuracy: 92.942%

Training recall: 89.291%

Training precision: 97.228%

Training f\_measure: 92.024%

dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

1/32

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

2013-11-4 18:6 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 82.140%

Testing recall: 58.793%

Testing precision: 80.261%

Testing f\_measure: 64.644%

Training accuracy: 77.135%

Training recall: 65.380%

Training precision: 86.056%

Training f\_measure: 72.293%

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_load\_All\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

%setup parameters

4 hidden

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-6; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 1; % enable plotting

2013-11-6 14:3 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 81.631%

Testing recall: 59.365%

Testing precision: 76.829%

Testing f\_measure: 62.847%

Training accuracy: 94.808%

Training recall: 94.837%

Training precision: 94.790%

Training f\_measure: 94.811%

Overfitting but if change to:

hiddenUnits=60;

batchsize=100;

numepochs=10000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-6; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

Training accuracy: 52.620%

Training recall: 87.709%

Training precision: 51.539%

Training f\_measure: 64.927%

Testing accuracy: 56.013%

Testing recall: 95.570%

Testing precision: 53.357%

Testing f\_measure: 68.481%

underfitting.

Nov3

dl8

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

1/30

2013-11-3 15:49 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

Testing AUC: 88.568%

Testing recall: 70.429%

Testing precision: 86.619%

Testing f\_measure: 72.734%

Training accuracy: 82.310%

Training recall: 79.985%

Training precision: 83.965%

Training f\_measure: 81.886%

1/64

Sending a stop signal to all the labs ... stopped.

2013-11-3 17:18 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 87.600%

Testing recall: 68.103%

Testing precision: 85.098%

Testing f\_measure: 71.421%

Training accuracy: 85.220%

Training recall: 81.625%

Training precision: 88.031%

Training f\_measure: 84.624%

1/256

2013-11-4 1:26 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.640%

Testing recall: 60.710%

Testing precision: 87.374%

Testing f\_measure: 64.927%

Training accuracy: 88.284%

Training recall: 82.347%

Training precision: 93.749%

Training f\_measure: 87.483%

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

%setup parameters

numberOFFeature=size(trainPO, 2);

hiddenUnits=20;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0; %default is 0

1/30

2013-11-3 22:45 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 80.318%

Testing recall: 50.541%

Testing precision: 79.633%

Testing f\_measure: 53.743%

Training accuracy: 69.020%

Training recall: 55.824%

Training precision: 78.607%

Training f\_measure: 65.039%

1/256

numberOFFeature=size(trainPO, 2);

hiddenUnits=20;

batchsize=100;

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0; %default is 0

2013-11-5 :21 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 84.767%

Testing recall: 65.295%

Testing precision: 85.476%

Testing f\_measure: 69.545%

Training accuracy: 74.234%

Training recall: 67.760%

Training precision: 78.076%

Training f\_measure: 72.346%

dl83

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

1/8

%setup parameters

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

Testing AUC: 84.754%

Testing recall: 70.032%

Testing precision: 81.093%

Testing f\_measure: 73.285%

Training accuracy: 83.889%

Training recall: 80.705%

Training precision: 86.747%

Training f\_measure: 83.169%

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.5; %default 0.2

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0.5; %default is 0

2013-11-4 4:25 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 86.844%

Testing recall: 59.550%

Testing precision: 82.551%

Testing f\_measure: 65.015%

Training accuracy: 80.465%

Training recall: 69.576%

Training precision: 89.120%

Training f\_measure: 76.081%

OCT31

dl82

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

1/8

Number of total DDI is: 30

Number of successed DDI is: 29

Number of total sequence is: 153

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 87.781%  
Testing recall: 59.727%

Testing precision: 77.661%

Testing f\_measure: 63.865%

Training accuracy: 91.046%

Training recall: 85.511%

Training precision: 96.686%

Training f\_measure: 89.617%

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DLUS', 'DLUS', 1, 1)

1/8

%setup parameters

numberOFFeature=size(test\_x, 2);

hiddenUnits=20;

batchsize=size(preTrain\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

plot = 0; % enable plotting

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DLUS Kernel: DLUS, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 87.599%

Testing recall: 69.171%

Testing precision: 84.996%

Testing f\_measure: 73.370%

Training accuracy: 84.189%

Training recall: 78.932%

Training precision: 88.448%

Training f\_measure: 82.607%

dl1

run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25('listOfDDIsHaveOver2InterfacesHave10-20ExamplesWithDifferentDomain.txt')

2013-11-1 12:40 SUCCESS: UreE\_C\_int\_UreE\_N2013-11-1 12:40 FINISHED.

>> =>> PBS: job killed: walltime 1080025 exceeded limit 1080000

OCT

dl8

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-6; %default 1.00e-3

learningRate= 0.01; %default is 1

dropoutFraction=0; %default is 0

2013-10-30 22:12 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.971%

Testing recall: 69.751%

Testing precision: 81.956%

Testing f\_measure: 71.549%

Training accuracy: 83.059%

Training recall: 82.608%

Training precision: 83.364%

Training f\_measure: 82.979%

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-30 1:56 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 84.002%

Testing recall: 69.415%

Testing precision: 78.755%

Testing f\_measure: 71.626%

Training accuracy: 95.205%

Training recall: 95.913%

Training precision: 94.668%

Training f\_measure: 95.232%

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=3000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-06; %default 1.00e-3

learningRate= 0.1; %default is 1

dropoutFraction=0; %default is 0

exploded.

OCT25

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'All', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.01;

scriptError correct it.

dl1

run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25('listOfDDIsHaveOver2InterfacesHave10-20ExamplesWithDifferentDomain.txt')

A lot didn't able to read ddi\_str\_array.mat

2013-10-26 8:55 SUCCESS: MHC\_II\_alpha\_int\_V-set2013-10-26 8:55 ERROR: MSP\_int\_Photo\_RC. Message: Unable to read file /home/du/Protein\_Protein\_Interaction\_Project/3did\_15OCT2010/topologyTest/dom\_dom\_ints/MSP\_int\_Photo\_RC/ddi\_str\_array.mat: No such file or directory.

redirect to /home/du/Protein\_Protein\_Interaction\_Project/3did\_15OCT2010/dom\_dom\_ints/

OCT24

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.05; %default is 1 if use 0.1 it will explode.

dropoutFraction=0; %default is 0

Training AUC: 91.324%

Training accuracy: 83.186%

Training recall: 82.462%

Training precision: 83.674%

Training f\_measure: 83.064%

Testing AUC: 91.960%

Testing accuracy: 84.177%

Testing recall: 92.405%

Testing precision: 79.348%

Testing f\_measure: 85.380%

2013-10-24 15:23 SUCCESS: PF00004.21\_int\_PF09336.2

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1', 'DL', 'DL', 1, 1)

Training AE 1/2

Training AE 2/2

Training AUC: 91.324%

Training accuracy: 83.186%

Training recall: 82.462%

Training precision: 83.674%

Training f\_measure: 83.064%

Testing AUC: 91.960%

Testing accuracy: 84.177%

Testing recall: 92.405%

Testing precision: 79.348%

Testing f\_measure: 85.380%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'All', 'DL', 'DL', 1, 1)

explode

OCT22

dl8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', ''SVMLIGHT', 'LINEAR', 1, 0)

2013-10-23 :17 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 0

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.561%

Testing recall: 75.442%

Testing precision: 2.463%

Testing f\_measure: 4.514%

Training accuracy: 89.615%

Training recall: 87.720%

Training precision: 91.264%

Training f\_measure: 89.109%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA3', ''SVMLIGHT', 'LINEAR', 1, 0)

dl1

run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25('listOfDDIsHaveOver2InterfacesHave10-20ExamplesWithDifferentDomain.txt')

error.

OCT21

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.1; %default is 1

dropoutFraction=0; %default is 0

Return NaN because learning rate too high and low weightpenaltyl2

hiddenUnits=30;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0; %default is 0

Training AE 1/2

Training AE 2/2

Training AUC: 91.593%

Training accuracy: 83.761%

Training recall: 85.449%

Training precision: 82.658%

Training f\_measure: 84.030%

Testing AUC: 92.021%

Testing accuracy: 83.861%

Testing recall: 94.304%

Testing precision: 78.010%

Testing f\_measure: 85.387%

numberOFFeature=size(train\_x, 2);

hiddenUnits=60;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.03; %default is 1

2013-10-23 18:29 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 115

Number of total sequence is: 115

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.762%

Testing recall: 77.663%

Testing precision: 87.209%

Testing f\_measure: 79.503%

Training AUC: 91.918%

Training accuracy: 84.121%

Training recall: 84.667%

Training precision: 83.766%

Training f\_measure: 84.206%

ContactMapsOn3DID\_2010\_new('listOfDDIsHaveOver2InterfacesHave10-20ExamplesWithDifferentDomain.txt')

dl8

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-22 2:12 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 56

Number of total sequence is: 56

FisherMode: FisherM1AA3 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.793%

Testing recall: 79.033%

Testing precision: 86.444%

Testing f\_measure: 79.385%

Training accuracy: 81.577%

Training recall: 83.986%

Training precision: 80.126%

Training f\_measure: 82.011%

With some error.

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-22 3:8 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 67

Number of total sequence is: 67

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.347%

Testing recall: 78.532%

Testing precision: 85.038%

Testing f\_measure: 78.231%

Training accuracy: 80.752%

Training recall: 84.409%

Training precision: 78.667%

Training f\_measure: 81.428%

With some error

OCT20

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.2; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.1; %default is 1

dropoutFraction=0; %default is 0

Number of total DDI is: 115

Number of successed DDI is: 115

Number of total sequence is: 115

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.840%

Testing recall: 78.180%

Testing precision: 88.108%

Testing f\_measure: 79.958%

Training accuracy: 85.527%

Training recall: 86.565%

Training precision: 84.899%

Training f\_measure: 85.670%

OCT19

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.2; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.1; %default is 1

dropoutFraction=0; %default is 0

Training AUC: 92.067%

Training accuracy: 84.212%

Training recall: 89.249%

Training precision: 81.080%

Training f\_measure: 84.969%

Testing AUC: 94.476%

Testing accuracy: 86.076%

Testing recall: 95.570%

Testing precision: 80.319%

Testing f\_measure: 87.283%

2013-10-19 16:22 SUCCESS: PF00004.21\_int\_PF09336.2.

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 1; %default is 1

dropoutFraction=0; %default is 0

Training AE 1/2

Training AE 2/2

Training AUC: 91.162%

Training accuracy: 82.363%

Training recall: 85.469%

Training precision: 80.470%

Training f\_measure: 82.894%

Testing AUC: 93.286%

Testing accuracy: 84.177%

Testing recall: 94.937%

Testing precision: 78.125%

Testing f\_measure: 85.714%

learning rate too high too much fluctuation.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.1; %default is 1

2013-10-21 11:9 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 115

Number of total sequence is: 115

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 93.316%

Testing recall: 77.383%

Testing precision: 87.327%

Testing f\_measure: 78.930%

Training accuracy: 83.485%

Training recall: 83.491%

Training precision: 83.568%

Dl8

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=1000;

inputZeroMaskedFraction=0.1; %default 0.5

weightPenaltyL2=1.00e-5; %default 1.00e-3

learningRate= 0.1; %default is 1

2013-10-20 10:18 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 115

Number of total sequence is: 115

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 57.423%

Testing recall: 48.647%

Testing precision: 55.831%

Testing f\_measure: 51.484%

Training accuracy: 58.337%

Training recall: 53.190%

Training precision: 59.244%

Training f\_measure: 55.954%

ContactMapsOn3DID\_2010('listOfDDIsHaveOver2InterfacesHave10-20ExamplesWithDifferentDomain.txt') error caused by pfam.pfam. Use new version.

OCT18

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.2; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.1; %default is 1

plot = 0; % enable plotting

2013-10-18 23:3 FINISHED.

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 50

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.428%

Testing recall: 75.606%

Testing precision: 88.564%

Testing f\_measure: 77.977%

Training accuracy: 85.844%

Training recall: 85.163%

Training precision: 86.414%

Training f\_measure: 85.738%

OCT 17

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

plot = 1; % enable plotting

2013-10-17 15:7 STARTED.

Training AE 1/2

Training AE 2/2

Training AUC: 87.659%

Training accuracy: 77.998%

Training recall: 75.458%

Training precision: 79.496%

Training f\_measure: 77.425%

Testing AUC: 95.145%

Testing accuracy: 85.443%

Testing recall: 93.038%

Testing precision: 80.769%

Testing f\_measure: 86.471%

2013-10-17 15:51 SUCCESS: PF00004.21\_int\_PF09336.2.

Underfitting.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=3000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

plot = 1; % enable plotting

2013-10-17 16:24 STARTED.

Training AE 1/2

Training AE 2/2

Training AUC: 87.669%

Training accuracy: 77.669%

Training recall: 76.175%

Training precision: 78.522%

Training f\_measure: 77.331%

Testing AUC: 91.744%

Testing accuracy: 81.962%

Testing recall: 95.570%

Testing precision: 75.124%

Testing f\_measure: 84.123%

After disable inputZeroMaskedFraction and change number of hidden units to 30 we still see underfitting. So Which means FisherM1Only is not enough for classification. So try FisherM1AA3.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

2013-10-17 17:30 STARTED.

Training AE 1/2

Training AE 2/2

Training AUC: 92.369%

Training accuracy: 84.980%

Training recall: 85.896%

Training precision: 84.351%

Training f\_measure: 85.116%

Testing AUC: 91.175%

Testing accuracy: 81.013%

Testing recall: 88.608%

Testing precision: 76.923%

Testing f\_measure: 82.353%

Should increase the number of epoch or increase training rate because the training error is still decreasing.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=5000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.1; %default is 1

Training AUC: 94.842%

Training accuracy: 89.572%

Training recall: 87.012%

Training precision: 91.707%

Training f\_measure: 89.298%

Testing AUC: 89.773%

Testing accuracy: 80.380%

Testing recall: 79.114%

Testing precision: 81.169%

Testing f\_measure: 80.128%

Should increase the number of epoch or increase training rate because the training error is still decreasing but the validation error is also increassing. Maybe add dropoutfraction to prevent overfitting.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=30;

batchsize=100;

numepochs=5000;

inputZeroMaskedFraction=0; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.1; %default is 1

dropoutFraction=0.5; %default is 0

2013-10-19 :51 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 89.761%

Testing recall: 69.889%

Testing precision: 87.826%

Testing f\_measure: 72.073%

Training accuracy: 79.299%

Training recall: 76.108%

Training precision: 81.308%

Training f\_measure: 78.613%

underfitting.

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

plot = 0; % enable plotting

2013-10-17 17: FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.269%

Testing recall: 70.944%

Testing precision: 87.331%

Testing f\_measure: 71.968%

Training accuracy: 78.356%

Training recall: 76.422%

Training precision: 79.502%

Training f\_measure: 77.929%

still underfitting

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1)

hiddenUnits=20;

batchsize=100;

numepochs=2000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

2013-10-17 19:25 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.581%

Testing recall: 71.858%

Testing precision: 88.204%

Testing f\_measure: 74.470%

Training accuracy: 83.039%

Training recall: 82.113%

Training precision: 83.688%

Training f\_measure: 82.876%

hiddenUnits=30;

batchsize=100;

numepochs=5000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.1; %default is 1

2013-10-18 :23 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1,

Testing AUC: 89.355%

Testing recall: 70.926%

Testing precision: 86.751%

Testing f\_measure: 74.268%

Training accuracy: 87.876%

Training recall: 87.456%

Training precision: 88.307%

Training f\_measure: 87.815%

OCT 16

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=100;

numepochs=10000;

inputZeroMaskedFraction=0.5; %default 0.5

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

plot = 1; % enable plotting

Training AUC: 87.683%

Training accuracy: 77.819%

Training recall: 75.896%

Training precision: 78.931%

Training f\_measure: 77.384%

Testing AUC: 95.145%

Testing accuracy: 86.076%

Testing recall: 94.937%

Testing precision: 80.645%

Testing f\_measure: 87.209%

2013-10-16 22:5 SUCCESS: PF00004.21\_int\_PF09336.2.

Looks good but I will kill it because the plotting take over the control.But underfitting

Oct15

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

2013-10-18 22:33 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.054%

Testing recall: 71.199%

Testing precision: 87.742%

Testing f\_measure: 72.335%

Training accuracy: 78.571%

Training recall: 76.446%

Training precision: 79.841%

Training f\_measure: 78.105%

Oct14

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-14 20:16 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 91.691%

Testing recall: 72.461%

Testing precision: 87.310%

Testing f\_measure: 73.885%

Training accuracy: 78.884%

Training recall: 78.096%

Training precision: 79.351%

Training f\_measure: 78.716%

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt', 'FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-15 16:46 FINISHED.

Number of total DDI is: 115

Number of successed DDI is: 86

Number of total sequence is: 86

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 92.993%

Testing recall: 78.810%

Testing precision: 85.391%

Testing f\_measure: 78.672%

Training accuracy: 80.789%

Training recall: 84.088%

Training precision: 78.883%

Training f\_measure: 81.402%

Oct12

local

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA3', 'DL', 'DL', 1, 1) %setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0.5;

FisherMode: FisherM1AA3 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 87.421%

Testing recall: 72.108%

Testing precision: 84.895%

Testing f\_measure: 75.876%

Training accuracy: 92.880%

Training recall: 91.861%

Training precision: 93.749%

Training f\_measure: 92.701%

Oct11

dl8

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'SVMLIGHT', 'LINEAR', 1, 1)

2013-10-11 20:31 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 30

FisherMode: FisherM1AA1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.654%

Testing recall: 71.767%

Testing precision: 87.937%

Testing f\_measure: 73.628%

Training accuracy: 79.399%

Training recall: 77.843%

Training precision: 80.345%

Training f\_measure: 79.073%

dl82

run3DID\_remote\_ChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'None', 'DL', 'DL', 1, 1)

2013-10-11 16:39 STARTED.

Training AUC: 52.614%

Training accuracy: 51.155%

Training recall: 69.562%

Training precision: 50.844%

Training f\_measure: 58.748%

Testing AUC: 50.813%

Testing accuracy: 48.101%

Testing recall: 65.190%

Testing precision: 48.585%

Testing f\_measure: 55.676%

2013-10-12 6:59 SUCCESS: PF00004.21\_int\_PF09336.2.

killed

screen -collect2

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote\_1('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'AAIndex3', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

killed. NoFor too good one hidden layer because few trying examples too many features.

Training accuracy: 85.714%

Training recall: 87.395%

Training precision: 84.553%

Training f\_measure: 85.950%

Testing accuracy: 75.000%

Testing recall: 83.333%

Testing precision: 71.429%

Testing f\_measure: 76.923%

Oct10

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=500000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.005; %default is 1

PF00004.21\_int\_PF09336.2

Training AE 2/2

Training accuracy: 97.872%

Training recall: 100.000%

Training precision: 95.918%

Training f\_measure: 97.917%

Testing accuracy: 74.219%

Testing recall: 67.188%

Testing precision: 78.182%

Testing f\_measure: 72.269%

Stopped because of clear overfitting. Use new settting add dropout.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=500000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.005; %default is 1

dropoutFraction=0.5; %default is 0

For one hidden layer

Training accuracy: 94.149%

Training recall: 98.936%

Training precision: 90.291%

Training f\_measure: 94.416%

Testing accuracy: 82.812%

Testing recall: 79.688%

Testing precision: 85.000%

Testing f\_measure: 82.258%

Stopped because of clear underfitting. Did not beat Oct6. Use new settting add dropout.

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

dropoutFraction=0.5;

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.479%

Testing recall: 74.113%

Testing precision: 85.829%

Testing f\_measure: 77.457%

Training accuracy: 90.148%

Training recall: 88.420%

Training precision: 91.470%

Training f\_measure: 89.762%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 1; %default is 1

2013-10-10 18:35 STARTED.

Training AE 1/1

For one hidden layer

Training accuracy: 78.367%

Training recall: 74.442%

Training precision: 80.783%

Training f\_measure: 77.483%

Testing accuracy: 88.291%

Testing recall: 94.937%

Testing precision: 83.799%

Testing f\_measure: 89.021%

Training AE 1/2

Training AE 2/2

Training accuracy: 50.000%

Training recall: 100.000%

Training precision: 50.000%

Training f\_measure: 66.667%

Testing accuracy: 50.000%

Testing recall: 100.000%

Testing precision: 50.000%

Testing f\_measure: 66.667%

Stopped because of explosion

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.03; %default is 1

2013-10-15 13:22 FINISHED.  
Number of total DDI is: 30  
Number of successed DDI is: 30  
Number of total sequence is: 30  
FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1  
The baseline AUC: 0.000%  
The baseline recall: 0.000%  
The baseline precision: 0.000%  
**Testing AUC: 92.468%**  
**Testing recall: 72.845%  
Testing precision: 90.027%**  
Testing f\_measure: 74.822%  
Training accuracy: 80.405%  
Training recall: 78.429%  
Training precision: 81.657%  
Training f\_measure: 80.009%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

2013-10-11 2:54 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.569%

Testing recall: 73.651%

Testing precision: 85.845%

Testing f\_measure: 77.092%

Training accuracy: 88.215%

Training recall: 84.600%

Training precision: 91.176%

Training f\_measure: 87.318%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote\_1('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

Oct8

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('testDDI.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

SUCCESS: PF00051.10\_int\_PF00051.10.

Testing recall: 54.192%

Testing precision: 71.736%

Testing f\_measure: 59.504%

Training accuracy: 96.094%

Training recall: 95.461%

Training precision: 96.720%

Training f\_measure: 96.072%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('testDDI.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=1000000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

SUCCESS: PF00051.10\_int\_PF00051.10.

Testing AUC: 76.147%

Testing recall: 60.188%

Testing precision: 84.742%

Testing f\_measure: 68.646%

Training accuracy: 92.098%

Training recall: 90.016%

Training precision: 94.015%

Training f\_measure: 91.909%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_cross('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

Stopped.

Oct7

inter

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL\_remote('list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-3; %default 1.00e-3

learningRate= 0.01; %default is 1

2013-10-11 :4 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 425

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 97.190%

Testing recall: 97.250%

Testing precision: 92.031%

Testing f\_measure: 94.243%

Training accuracy: 94.768%

Training recall: 97.862%

Training precision: 92.589%

Training f\_measure: 95.066%

Oct6

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=1.00e-4; %default 1.00e-3

learningRate= 0.01; %default is 1

2013-10-8 :52 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 89.369%

Testing recall: 77.102%

Testing precision: 84.396%

Testing f\_measure: 79.129%

Training accuracy: 95.234%

Training recall: 95.624%

Training precision: 94.930%

Training f\_measure: 95.256%

With current learning rate some DDI exploded.

Oct4

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0.2; %default 0.2

weightPenaltyL2=0; %default 1.00e-3

learningRate= 0.003; %default is 1

2013-10-6 :29 FINISHED.

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.464%

Testing recall: 74.820%

Testing precision: 84.075%

Testing f\_measure: 77.348%

Training accuracy: 90.084%

Training recall: 89.279%

Training precision: 90.667%

Training f\_measure: 89.899%

Oct4 updated

ContactMapsOn3DID\_2010('listOfSuccessCopied\_listOfDDIWithSingleTop10to20Examples.txt')

run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25('listOfSuccessCopied\_listOfDDIWithSingleTop10to20Examples.txt')

generate

Done

list\_of\_SUCCESS\_aaIndex\_topology\_Sep25\_10\_to 20\_lessThan150\_30.txt

Oct2

Oct1

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1ONLY', 'DL', 'DL', 1, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 88.167%

Testing recall: 71.007%

Testing precision: 83.663%

Testing f\_measure: 74.930%

Training accuracy: 84.368%

Training recall: 77.559%

Training precision: 89.401%

Training f\_measure: 82.407%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('testDDI.txt', 'FisherM1AA1', 'DL', 'DL', 10, 10)

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 10, choseNegRatioTest: 10

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 90.888%

Testing recall: 48.186%

Testing precision: 91.667%

Testing f\_measure: 61.098%

Training accuracy: 95.223%

Training recall: 48.839%

Training precision: 95.906%

Training f\_measure: 63.298%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('testDDI.txt', 'FisherM1AA1', 'DL', 'DL', 0, 0)

Training AE 1/1

For one hidden layer

Training accuracy: 99.873%

Training recall: 0.000%

Training precision: 0.000%

Training f\_measure: 0.000%

Testing accuracy: 99.897%

Testing recall: 0.000%

Testing precision: 0.000%

Testing f\_measure: 0.000%

Training AE 1/2

Training AE 2/2

Training accuracy: 99.873%

Training recall: 0.000%

Training precision: 0.000%

Training f\_measure: 0.000%

Testing accuracy: 99.897%

Testing recall: 0.000%

Testing precision: 0.000%

Testing f\_measure: 0.000%

Sep 30

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('testDDI.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0; %default 0.2

weightPenaltyL2=0; %default 1.00e-3

learningRate= 0.001; %default is 1

2013-9-30 19:35 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 4

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 96.448%

Testing recall: 86.213%

Testing precision: 89.899%

Testing f\_measure: 87.899%

Training accuracy: 87.946%

Training recall: 90.094%

Training precision: 86.407%

Training f\_measure: 88.161%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_DL('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt', 'FisherM1AA1', 'DL', 'DL', 1, 1)

%setup parameters

numberOFFeature=size(train\_x, 2);

hiddenUnits=20;

batchsize=size(train\_x, 1);

numepochs=100000;

inputZeroMaskedFraction=0; %default 0.2

weightPenaltyL2=0; %default 1.00e-3

learningRate= 0.001; %default is 1

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1AA1 SVMMode: DL Kernel: DL, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 0.000%

The baseline recall: 0.000%

The baseline precision: 0.000%

Testing AUC: 85.171%

Testing recall: 73.098%

Testing precision: 81.196%

Testing f\_measure: 74.915%

Training accuracy: 84.727%

Training recall: 82.117%

Training precision: 86.281%

Training f\_measure: 83.939%

Sep26

screen -r con3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1, 0.000001, 1 )

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-06 J: 1

The baseline AUC: 73.532%

The baseline recall: 47.643%

The baseline precision: 69.825%

Testing AUC: 83.242%

Testing recall: 43.252%

Testing precision: 63.128%

Testing f\_measure: 47.682%

Training accuracy: 99.999%

Training recall: 100.000%

Training precision: 99.998%

Training f\_measure: 99.999%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1, 0.0000000001, 1 )

Number of total DDI is: 30  
Number of successed DDI is: 30  
Number of total sequence is: 155  
FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-10 J: 1  
The baseline AUC: 73.321%  
The baseline recall: 47.643%  
The baseline precision: 69.546%  
Testing AUC: 82.700%  
Testing recall: 26.907%  
Testing precision: 55.608%  
Testing f\_measure: 31.352%  
Training accuracy: 83.799%  
Training recall: 69.037%  
Training precision: 99.101%  
Training f\_measure: 78.477%

screen -r con1

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 3, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 3, choseNegRatioTest: 1

The baseline AUC: 73.429%

The baseline recall: 47.643%

The baseline precision: 69.548%

Testing AUC: 84.570%

Testing recall: 51.962%

Testing precision: 78.606%

Testing f\_measure: 59.104%

Training accuracy: 94.231%

Training recall: 82.783%

Training precision: 93.579%

Training f\_measure: 87.149%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1AA1', 'SVMLIGHT', 'LINEAR', 1, 1)

FisherMode: FisherM1AA1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1  
The baseline AUC: 73.523%  
The baseline recall: 47.643%  
The baseline precision: 69.653%  
Testing AUC: 87.694%  
Testing recall: 74.972%  
Testing precision: 82.641%  
Testing f\_measure: 76.712%  
Training accuracy: 90.121%  
Training recall: 89.334%  
Training precision: 90.863%  
Training f\_measure: 89.859%

Sep 25

On biohen

screen -r con1

inter341

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1, 0.01, 1 )

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-02 J: 1

The baseline AUC: 73.532%

The baseline recall: 47.643%

The baseline precision: 69.631%

Testing AUC: 82.704%

Testing recall: 69.792%

Testing precision: 76.843%

Testing f\_measure: 71.642%

Training accuracy: 97.777%

Training recall: 98.531%

Training precision: 97.125%

Training f\_measure: 97.809%

screen -r con2

inter341

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1, 0.1, 1 )

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-01 J: 1

The baseline AUC: 73.532%

The baseline recall: 47.643%

The baseline precision: 69.631%

Testing AUC: 81.746%

Testing recall: 68.463%

Testing precision: 75.146%

Testing f\_measure: 70.290%

Training accuracy: 99.548%

Training recall: 99.773%

Training precision: 99.354%

Training f\_measure: 99.559%

screen -r con3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1, 0.001, 1 )

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-03 J: 1

The baseline AUC: 76.383%

The baseline recall: 53.184%

The baseline precision: 73.583%

Testing AUC: 84.828%

Testing recall: 43.282%

Testing precision: 63.785%

Testing f\_measure: 47.338%

Training accuracy: 99.995%

Training recall: 99.997%

Training precision: 99.993%

Training f\_measure: 99.995%

screen -r collect

inter341

run3DID\_CellectVectors\_Fishers\_aaIndex\_Sep12('finishedDDIs\_ContinuedSep25.txt')

update run3DID\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25.m

runSeqPair\_CellectVectors\_Fishers\_aaIndex\_topology\_Sep25.m ContactMapsOn3DID\_2010(file\_ddis).m do not do clustering.

Sep 23

screen -r con1

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1, 0.001, 1 )

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-03 J: 1

The baseline AUC: 73.545%

The baseline recall: 47.643%

The baseline precision: 69.775%

Testing AUC: 82.531%

Testing recall: 66.797%

Testing precision: 78.876%

Testing f\_measure: 69.703%

Training accuracy: 91.647%

Training recall: 90.928%

Training precision: 92.423%

Training f\_measure: 91.488%

screen -r con2

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1, 0.0001, 1 )

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-04 J: 1

The baseline AUC: 73.430%

The baseline recall: 47.643%

The baseline precision: 69.390%

Testing AUC: 82.174%

Testing recall: 58.793%

Testing precision: 78.014%

Testing f\_measure: 63.323%

Training accuracy: 87.062%

Training recall: 81.612%

Training precision: 92.198%

Training f\_measure: 85.702%

screen -r con3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1, 0.00001, 1 )

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-05 J: 1

The baseline AUC: 73.580%

The baseline recall: 47.643%

The baseline precision: 69.805%

Testing AUC: 81.250%

Testing recall: 57.775%

Testing precision: 76.856%

Testing f\_measure: 62.122%

Training accuracy: 86.613%

Training recall: 80.965%

Training precision: 92.441%

Training f\_measure: 85.364%

screen -r con4

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR',FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-06 J: 1

The baseline AUC: 73.584%

The baseline recall: 47.643%

The baseline precision: 68.953%

Testing AUC: 82.797%

Testing recall: 58.940%

Testing precision: 75.293%

Testing f\_measure: 61.559%

Training accuracy: 84.204%

Training recall: 81.175%

Training precision: 89.331%

Training f\_measure: 83.451%

Sep 22

screen -r con1

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1, 0.001, 1 )

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-03 J: 1

The baseline AUC: 73.455%

The baseline recall: 47.643%

The baseline precision: 69.677%

Testing AUC: 84.943%

Testing recall: 68.945%

Testing precision: 80.064%

Testing f\_measure: 71.742%

Training accuracy: 92.627%

Training recall: 92.073%

Training precision: 93.272%

Training f\_measure: 92.494%

screen -r con2

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1, 0.0001, 1 )

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-04 J: 1

The baseline AUC: 73.456%

The baseline recall: 47.643%

The baseline precision: 69.671%

Testing AUC: 82.906%

Testing recall: 60.504%

Testing precision: 75.502%

Testing f\_measure: 63.324%

Training accuracy: 85.564%

Training recall: 78.580%

Training precision: 92.634%

Training f\_measure: 82.676%

screen -r con3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1, 0.00001, 1 )

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-05 J: 1

The baseline AUC: 73.492%

The baseline recall: 47.643%

The baseline precision: 69.865%

Testing AUC: 83.871%

Testing recall: 61.456%

Testing precision: 76.392%

Testing f\_measure: 64.318%

Training accuracy: 85.368%

Training recall: 78.418%

Training precision: 92.497%

Training f\_measure: 82.257%

screen -r con4

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load\_C\_J('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1, 0.000001, 1 )

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1 C: 1.000000e-06 J: 1

The baseline AUC: 73.409%

The baseline recall: 47.643%

The baseline precision: 69.280%

Testing AUC: 82.163%

Testing recall: 60.014%

Testing precision: 71.309%

Testing f\_measure: 60.369%

Training accuracy: 82.383%

Training recall: 77.802%

Training precision: 89.307%

Training f\_measure: 79.766%

Sep 18

The value *C* is called the Error Penalty. A high error penalty will force the SVM training to avoid classification errors

Setting default regularization parameter C=0.0031 for LINEAR

Setting default regularization parameter C=0.0000 for POLY

Mel screen -S con1

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 73.583%

The baseline recall: 47.643%

The baseline precision: 69.552%

Testing AUC: 84.066%

Testing recall: 69.457%

Testing precision: 78.737%

Testing f\_measure: 71.457%

Training accuracy: 95.479%

Training recall: 96.297%

Training precision: 94.820%

Training f\_measure: 95.515%

Why this is lower than expected.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 76.262%

The baseline recall: 53.184%

The baseline precision: 73.892%

Testing AUC: 84.419%

Testing recall: 70.634%

Testing precision: 79.177%

Testing f\_measure: 72.377%

Training accuracy: 96.032%

Training recall: 96.994%

Training precision: 95.233%

Training f\_measure: 96.074%

screen -S con2

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

Setting default regularization parameter C=0.0663

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 73.523%

The baseline recall: 47.643%

The baseline precision: 69.653%

Testing AUC: 90.702%

Testing recall: 76.844%

Testing precision: 86.053%

Testing f\_measure: 78.485%

Training accuracy: 89.579%

Training recall: 88.073%

Training precision: 90.984%

Training f\_measure: 89.204%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 76.375%

The baseline recall: 53.184%

The baseline precision: 73.575%

Testing AUC: 91.291%

Testing recall: 76.818%

Testing precision: 84.553%

Testing f\_measure: 78.623%

Training accuracy: 91.052%

Training recall: 90.168%

Training precision: 91.906%

Training f\_measure: 90.736%

screen -S con3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 73.532%

The baseline recall: 47.643%

The baseline precision: 70.137%

Testing AUC: 85.021%

Testing recall: 71.979%

Testing precision: 81.204%

Testing f\_measure: 73.972%

Training accuracy: 95.415%

Training recall: 96.092%

Training precision: 94.928%

Training f\_measure: 95.451%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1)

Setting default regularization parameter C=0.0031

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: All SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 76.417%

The baseline recall: 53.184%

The baseline precision: 74.152%

Testing AUC: 86.968%

Testing recall: 73.222%

Testing precision: 81.645%

Testing f\_measure: 74.787%

Training accuracy: 96.341%

Training recall: 96.942%

Training precision: 95.851%

Training f\_measure: 96.362%

screen -S con4

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1)

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 73.519%

The baseline recall: 47.643%

The baseline precision: 69.929%

Testing AUC: 82.560%

Testing recall: 41.366%

Testing precision: 62.555%

Testing f\_measure: 46.190%

Training accuracy: 99.455%

Training recall: 98.935%

Training precision: 99.976%

Training f\_measure: 99.444%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1)

Setting default regularization parameter C=0.0000

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 76.298%

The baseline recall: 53.184%

The baseline precision: 73.437%

Testing AUC: 84.925%

Testing recall: 43.399%

Testing precision: 64.183%

Testing f\_measure: 47.820%

Training accuracy: 99.300%

Training recall: 98.689%

Training precision: 99.914%

Training f\_measure: 99.283%

screen -S con5

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011\_30.txt','FisherM1ONLY', 'SVMLIGHT', 'POLY', 1, 1)

Setting default regularization parameter C=0.0001

Number of total DDI is: 30

Number of successed DDI is: 30

Number of total sequence is: 155

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 73.532%

The baseline recall: 47.643%

The baseline precision: 69.631%

Testing AUC: 89.222%

Testing recall: 56.531%

Testing precision: 79.232%

Testing f\_measure: 62.890%

Training accuracy: 84.478%

Training recall: 72.066%

Training precision: 96.480%

Training f\_measure: 80.228%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1ONLY', 'SVMLIGHT', 'POLY', 1, 1)

Number of total DDI is: 50

Number of successed DDI is: 50

Number of total sequence is: 238

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 76.315%

The baseline recall: 53.184%

The baseline precision: 73.803%

Testing AUC: 90.399%

Testing recall: 58.292%

Testing precision: 79.802%

Testing f\_measure: 64.286%

Training accuracy: 86.748%

Training recall: 76.237%

Training precision: 97.170%

Training f\_measure: 83.556%

Sep 17

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 3, 1)

2013-9-18 13:28 FINISHED.

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 3

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 3, choseNegRatioTest: 1

The baseline AUC: 89.199%

The baseline recall: 78.774%

The baseline precision: 99.242%

Testing AUC: 92.957%

Testing recall: 62.538%

Testing precision: 84.290%

Testing f\_measure: 67.102%

Training accuracy: 92.272%

Training recall: 86.622%

Training precision: 83.258%

Training f\_measure: 84.861%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM1ONLY', 'SVMLIGHT', 'LINEAR', 1, 1)

Number of total DDI is: 1

Number of successed DDI is: 1

Number of total sequence is: 3

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.387%

The baseline recall: 78.774%

The baseline precision: 100.000%

Testing AUC: 93.463%

Testing recall: 59.435%

Testing precision: 90.143%

Testing f\_measure: 60.111%

Training accuracy: 92.117%

Training recall: 95.749%

Training precision: 89.303%

Training f\_measure: 92.383%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM1ONLY', 'SVMLIGHT', 'POLY', 1, 1)

FisherMode: FisherM1ONLY SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 88.938%

The baseline recall: 78.774%

The baseline precision: 99.020%

Testing AUC: 91.092%

Testing recall: 58.975%

Testing precision: 86.919%

Testing f\_measure: 63.235%

Training accuracy: 91.548%

Training recall: 88.848%

Training precision: 93.813%

Training f\_measure: 91.241%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM1', 'SVMLIGHT', 'POLY', 1, 1)

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: POLY, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.387%

The baseline recall: 78.774%

The baseline precision: 100.000%

Testing AUC: 94.450%

Testing recall: 28.827%

Testing precision: 100.000%

Testing f\_measure: 43.499%

Training accuracy: 100.000%

Training recall: 100.000%

Training precision: 100.000%

Training f\_measure: 100.000%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 1, 1)

FisherMode: FisherM1 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.387%

The baseline recall: 78.774%

The baseline precision: 100.000%

Testing AUC: 94.310%

Testing recall: 76.336%

Testing precision: 90.128%

Testing f\_measure: 81.684%

Training accuracy: 97.006%

Training recall: 98.742%

Training precision: 95.437%

Training f\_measure: 97.060%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','FisherM0', 'SVMLIGHT', 'LINEAR', 1, 1)

FisherMode: FisherM0 SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.216%

The baseline recall: 78.774%

The baseline precision: 99.320%

Testing AUC: 87.720%

Testing recall: 81.439%

Testing precision: 79.718%

Testing f\_measure: 80.477%

Training accuracy: 93.453%

Training recall: 97.259%

Training precision: 90.405%

Training f\_measure: 93.684%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','None', 'SVMLIGHT', 'LINEAR', 1, 1)

FisherMode: None SVMMode: SVMLIGHT Kernel: LINEAR, choseNegRatio: 1, choseNegRatioTest: 1

The baseline AUC: 89.011%

The baseline recall: 78.774%

The baseline precision: 98.519%

Testing AUC: 79.622%

Testing recall: 65.338%

Testing precision: 71.966%

Testing f\_measure: 68.269%

Training accuracy: 92.596%

Training recall: 93.851%

Training precision: 91.549%

Training f\_measure: 92.686%

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test\_load('testDDI.txt','All', 'SVMLIGHT', 'LINEAR', 1, 1)

run3DID\_CellectVectors\_Fishers\_aaIndex\_Sep12('finishedDDIs\_ContinuedSep17.txt')

Sep 13

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt', 'FisherM1', 'SVMLIGHT', 'POLY', 1)

Mel is down.

Sep 12

modify run3DID\_CellectVectors\_Fishers\_aaIndex.m to run3DID\_CellectVectors\_Fishers\_aaIndex\_Sep12(file\_ddis)

%For each sequence, build a matrix index by the sequence number. I decided to write it to different DDI direcoty instead of just one big file. No longer write training and validation set.

%outputPath=['/big/du/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project/Vectors\_Fishers\_aaIndex\_raw/' ddiddiName '/']

run3DID\_CellectVectors\_Fishers\_aaIndex\_Sep12('showcaseDDI\_05NOV2011.txt')

test OK.

on Mel

run3DID\_CellectVectors\_Fishers\_aaIndex\_Sep12('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt')

mel is down.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test( 'showcaseDDI\_05NOV2011.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR', 1)

ERROR: PF00025.13\_int\_PF00025.13. Message: This DDI was taking too long.

Aug 06 2012

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('log\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_LINEAR\_06AUG2013.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 'Aug8')

But this result was from the wrong script. Which did not use the trainning data to write the model file, but use the old svm model file. But the result is good. Need to find out which script wrote the model file. Mddel file was the old one. It was find out the file was writen on Jul 3 00:25 /PF00019.12\_int\_PF07686.9/.

The problem of the good performance is that it use the model file of POLY and classify as linear classifier. Model from the following script. On JUNE 28

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('FisherM1', 'SVMLIGHT', 'POLY').

And the POLY use much more regularization Setting

default regularization parameter C=0.0000

-rwxr-xr-x 1 du cwu 112158 Jul 3 00:25 FisherM1\_AllVectorsChooseNegRand\_02NOV2011.model

-rwxr-xr-x 1 du cwu 208503 Aug 18 23:03 FisherM1\_AllVectorsChooseNegRand\_02NOV2011.test

-rwxr-xr-x 1 du cwu 109690 Aug 18 22:54 FisherM1\_AllVectorsChooseNegRand\_02NOV2011.train

The total number of DDIs is: 115

The total number of successed DDIs is: 109

The number of training sequence pairs LOO is: 434

average AUC is: 0.962287

average Recall is: 0.853238

average Precision is: 0.883490

average baseline AUC is: 0.788481

average baseline Recall is: 0.582230

average baseline Precision is: 0.800103

July8

Create

on biohen

run3DID\_AllVectorsAllNeg\_P8\_aaIndex\_test.m

run3DID\_AllVectorsAllNeg\_P8\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR')

July 3

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR')

run3DID\_CellectVectors\_Fishers\_aaIndex('showcaseDDI\_05NOV2011.txt')

July4

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1', 'SVMLIGHT', 'POLY', 'July4')

Using wrong old model file

python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_July4.txt number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_July4.txt:238

The total number of DDIs is 50

The number of training sequence pairs LOO is 238

The number of average SVM AUC is 0.859803

The number of average SVM Recall is 0.498643

The number of average SVM Precision is 0.711395

The number of average baseline AUC is 0.764034

The number of average baseline Recall is 0.531840

The number of average baseline Precision is 0.738895

This is not accurate only 9 success.

Rerun it.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt', 'FisherM1', 'SVMLIGHT', 'LINEAR')

JULY 7

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_test\_50.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 'July7')

python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_LINEAR\_July7.txt

python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_LINEAR\_July7.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_LINEAR\_July7.txt:186

The total number of DDIs is 50

The number of training sequence pairs LOO is 186

The number of average SVM AUC is 0.958403

The number of average SVM Recall is 0.833081

The number of average SVM Precision is 0.862839

The number of average baseline AUC is 0.755414

The number of average baseline Recall is 0.516204

The number of average baseline Precision is 0.733387

JULY8

modified reportResultsAllVectorsChooseNegRand\_aaIndex\_test.m to take logfile

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('log\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_LINEAR\_04JUL2013.txt','FisherM1', 'SVMLIGHT', 'LINEAR', 'July8')

The total number of DDIs is: 50

The total number of successed DDIs is: 34

The number of training sequence pairs LOO is: 148

average AUC is: 0.960589

average Recall is: 0.850644

average Precision is: 0.850644

average baseline AUC is: 0.730014

average baseline Recall is: 0.466743

average baseline Precision is: 0.678739

JUNE 28

modified functions

function V=getAAindexVector(seqence, location, WINDOW)

and runSeqPairAllVectorsChooseNegRand\_aaIndex\_test.m to calculate the 5 sliding window as input.

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('FisherM1', 'SVMLIGHT', 'POLY').

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('FisherM1', 'SVMLIGHT', 'POLY', 'June28')

generate resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June22.txt

python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June28.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June28.txt:473

The total number of DDIs is 115

The number of training sequence pairs LOO is 473

The number of average SVM AUC is 0.879108

The number of average SVM Recall is 0.525689

The number of average SVM Precision is 0.745207

The number of average baseline AUC is 0.782279

The number of average baseline Recall is 0.569175

The number of average baseline Precision is 0.783558 Sad adding more features lower the performance. Over fitting.

June27

Sending a stop signal to all the labs ... stopped.

2013-6-26 9:49 FINISHED.

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June22.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June22.txt:473

The total number of DDIs is 115

The number of training sequence pairs LOO is 473

The number of average SVM AUC is 0.884209

The number of average SVM Recall is 0.597070

The number of average SVM Precision is 0.825643

The number of average baseline AUC is 0.782649

The number of average baseline Recall is 0.569175

The number of average baseline Precision is 0.783040

On June 22 2013

Create

run3DID\_AllVectorsChooseNegRand\_aaIndex\_test.m

runSeqPairAllVectorsChooseNegRand\_aaIndex\_test.m

in this file new way to generate rand negative examples.

indTrainNE = randi([1 size(FamilyNE, 1)], numbNegTrain, 1);

whileTimer1 = clock;

while length(unique(indTrainNE)) < length(indTrainNE)

indTrainNE = randi([1 size(FamilyNE, 1)], numbNegTrain, 1);

whileET = etime(clock, whileTimer1);

if whileET > 4\*60

error('took too long to find unique train negative examples.');

end

end

TO:

r=randperm(size(FamilyNE, 1));

r=r(1:numbNegTrain)

FamilyNE = FamilyNE(r, :);

for i=1:length(posTestI)

POTest = [POTest;

ATestFisherVectors(posTestI(i), :) getAAindexVector(conservedProteinSequenceA, posTestI(i)) ...

BTestFisherVectors(posTestJ(i), :) getAAindexVector(conservedProteinSequenceB, posTestJ(i)) ];

end

On mel: run3DID\_AllVectorsChooseNegRand\_aaIndex\_test('FisherM1', 'SVMLIGHT', 'POLY') with 17 Aaindex.

reportResultsAllVectorsChooseNegRand\_aaIndex\_test('FisherM1', 'SVMLIGHT', 'POLY', 'June22') first 50.

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June22.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June22.txt:238

The total number of DDIs is 50

The number of training sequence pairs LOO is 238

The number of average SVM AUC is 0.874492

The number of average SVM Recall is 0.592782

The number of average SVM Precision is 0.816643

The number of average baseline AUC is 0.763071

The number of average baseline Recall is 0.531840

The number of average baseline Precision is 0.738811

On June 17 2013

reportResultsAllVectorsChooseNegRand\_02NOV2011('FisherM1', 'SVMLIGHT', 'POLY', 'June13')

generate: resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June13.txt

michael@OptiPlex-9010:~/Dropbox/Project/Contact\_maps$ python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June13.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_June13.txt:473

The total number of DDIs is 115

The number of training sequence pairs LOO is 473

The number of average SVM AUC is 0.910017

The number of average SVM Recall is 0.601416

The number of average SVM Precision is 0.817249

The number of average baseline AUC is 0.782814

The number of average baseline Recall is 0.569175

The number of average baseline Precision is 0.786495

Slightly Different from alvaro's because of the random negative part.

On June 13 2013

Problem. Clustering result only about 5 examples for each DDI

michael@OptiPlex-9010:~/Dropbox/Project/Contact\_maps$ python STAT\_reportResults\_02NOV2011.py resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt

number of lines in resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt:473

The total number of DDIs is 115

The number of training sequence pairs LOO is 473

The number of average SVM AUC is 0.911994

The number of average SVM Recall is 0.599004

The number of average SVM Precision is 0.826237

The number of average baseline AUC is 0.781076

The number of average baseline Recall is 0.569175

The number of average baseline Precision is 0.778414

re run on my diretory: run3DID\_AllVectorsChooseNegRand\_02NOV2011('FisherM1', 'SVMLIGHT', 'POLY')

On June 12 2013

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ cp ../Contact\_Matrix\_Project\_alvaro/run3DID\_AllVectorsChooseNegRand\_02NOV2011.m ./

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ cp ../Contact\_Matrix\_Project\_alvaro/finishedDDIs\_AllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt ./

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ cp ../Contact\_Matrix\_Project\_alvaro/runDDIAllVectorsChooseNegRand\_02NOV2011.m ./

du@melpomene ~/Protein\_Protein\_Interaction\_Project/Contact\_Matrix\_Project $ cp ../Contact\_Matrix\_Project\_alvaro/reportResultsAllVectorsChooseNegRand\_02NOV2011.m ./

Modify path accordingly.

In runDDIAllVectorsChooseNegRand\_02NOV2011(FisherMode, SVMMode, Kernel)) it will work clustered data.

reportResultsAllVectorsChooseNegRand\_02NOV2011('FisherM1', 'SVMLIGHT', 'POLY', '02NOV2011')

generate resultsAllVectorsChooseNegRand\_FisherM1\_SVMLIGHT\_POLY\_02NOV2011.txt

On June 11 2013

ContactMapsOn3DID('showcaseDDI\_05NOV2011.txt') write contactMactrix contactMapsBag.mat in to following folder.

cp . ./Contact\_Matrix\_Project\_alvaro/ContactMapExamples/ .

Rename Contact\_Matrix\_Project/ to Contact\_Matrix\_Project\_alvaro/

copy ContactMapsOn3DID.m from Contact\_Matrix\_Project\_alvaro/ and modify it accordingly and make it to to take DDI filename as input.

I.e.

ContactMapsOn3DID('showcaseDDI\_05NOV2011.txt')

Note: so before contactMap I need to build dataset and run clustering script which is not mentioned in alvaro's email(it will write the MC.mat in the folder). load([ddiPath 'MC' num2str(percThr) '.mat']);

Note: in this script it work on the whole data set, not just the clustered paires, But the clustered data can be obtained by the above note.

Showing figure in this script should be turned off when batch mode.