Expression Predictor Quick Start Guide



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1.1 Training/Testing Set Validation Over a Single Run

- 1. Double click on ExP.bat
- 2. Click on Project and select Load Data

Expression Predictor	_ []
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3. Select Input file

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1	p30s11_s	Wyeth	-		140.	Gumpic	Eaber
2 3	p30s16_s p30s28_s	Wyeth Wyeth	-11				
4	p30s20_s	Wyeth		Insert >>			
5	p30s29_s	Wyeth		<< Remove			
6	p30s41_s	Wyeth					
7 8	p30s09_s p30s13_s	Clofibrate Clofibrate					
9	p30s15_s	Clofibrate					
10	p30s14_s	Clofibrate		Testing Set			
11	p30s26_s	Clofibrate		1	No.	Sample	Label
12	p30s40_s p30s19_s	Clofibrate Gemfibrozil	-11		140.	Dample	Laber
14	p30s47_s	Gemfibrozil					
15	p30s48_s	Gemfibrozil		Insert >>			
16 17	p30s20_s p30s49_s	Gemfibrozil Gemfibrozil		<< Remove			
18	p30s49_s	Gemfibrozil					
					1		
19 20	p30s22_s p30s34_s	Phenobarbital Phenobarbital					

Submit

5. Select the Training set

FuzzyArtMapSample.txt g/Testing Set ု Leave		ation	Apply All Values	in Vigilan	ce Spectrun	n		
0.1 0.2	0.3 0.4	0.5	0.6	0.7	0.8	0.9	1.0	
Selection								
			Training Set					
Sample	Label				No		Pampia	Label
p30s09_s	Clofibrate	-			INO.		Gample	Label
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			<< Remove					
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xpression Predictor							_
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lidation: 💿 Training	/Testing Set 🛛 Leave	One Out Cross Validatio	n 🔄 Apply All Values in Vig	ilance Spectrun	n		
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			\bigcirc				
		0.3 0.4	0.5 0.6 0.7	0.8	0.9 1.0		
		0.5 0.4	0.0 0.1	0.0	0.5 1.0		
aining/Testing Set Se	election						
Original Set			Training Set				
-							
No. 25	Sample p30s10_s	Label Wyeth		No.	Sample	Label	
26	p30s15_s	Wyeth	2		p30s11_s	Wyeth	-
27	p30s15_s	Wyeth			p30s16_s p30s28_s	Wyeth Wyeth	
28	p30s08_s	Clofibrate	Insert >> 3 4			Wyeth	
29	p30s24_s	Clofibrate	<remove 5<="" td=""><td></td><td>p30s17_s p30s29_s</td><td>Wyeth</td><td>_</td></remove>		p30s17_s p30s29_s	Wyeth	_
30	p30s39_s	Clofibrate	S			Wyeth	_
31	p30s18_s	Gemfibrozil	- 0		p30s41_s	Clofibrate	_
32	p30s45_s	Gemfibrozil	- 8		p30s09_s p30s13_s	Clofibrate	
33	p30s46_s	Gemfibrozil			honero"e	Ciolibrate	-
34	p30s21_s	Phenobarbital	Testing Set				
35	p30s42_s	Phenobarbital	Testing Set				
36	p30s51_s	Phenobarbital		No.	Sample	Label	
	[p00001_0	THORODANDIA					
			Insert >>				
			<< Remove				
			Submit				

7. Select the Testing Set

	e\FuzzyArtMapSample.txt ing/Testing Set ု Leave	One Out Cross Validati	on 🗌 Apply All Values ir) Vigilance Spectrum	1		
0.0		0.3 0.4		0.7 0.8	0.5 0.9 1.0		
aining/Testing Set Original Set	Selection		Tanining Cat				
			Training Set				
No.	Sample	Label		No.	Sample	Label	
25	p30s10_s	Wyeth		1	p30s11_s	Wyeth	-
26	p30s15_s	Wyeth		2	p30s16_s	Wyeth	_
27	p30s27_s	Wyeth	Insert >>	3	p30s28_s	Wyeth	
28	p30s08_s	Clofibrate		4	p30s17_s	Wyeth	
29	p30s24_s	Clofibrate	<< Remove	5	p30s29_s	Wyeth	
30	p30s39_s	Clofibrate		6	p30s41_s	Wyeth	
31	p30s18_s	Gemfibrozil		7	p30s09_s	Clofibrate	
32	p30s45_s	Gemfibrozil		8	p30s13_s	Clofibrate	-
33	p30s46_s	Gemfibrozil					
34	p30s21_s	Phenobarbital	Testing Set				
35 36	p30s42_s p30s51_s	Phenobarbital Phenobarbital		No.	Sample	Label	_
		, nonobalinar	Insert >> << Remove				
			Submit				

8. Click on the "Insert>>" button on the Testing Set Panel

expression Predictor						_
ect						
Des Partient						
arameters Prediction						
e: D:\Demo\Sample\FuzzyArtMapSample	ixt					
alidation: 💿 Training/Testing Set 🛛 🔾	ave One Out Cross Validat	tion 📃 Apply All Values	in Vigilance Spectrum	1		
		,				
		_				
gilance:		-				
gliance: 0.0 0.1 0.2	0.3 0.4	0.5 0.6	0.7 0.8	0.9 1.0		
	010 011	010 010	010	010 110		
aining/Testing Set Selection						
Original Set		Training Set				
	1.1.1					
No. Sample	Label		No.	Sample	Label	_
			2	p30s11_s p30s16_s	Wyeth Wyeth	-
			3	p30s16_s	Wyeth	
		Insert >>	4	p30s28_s	Wyeth	
		<< Remove	5	p30s17_s	Wyeth	_
		<< Remove			Wyeth	_
			7	p30s41_s p30s09_s	Clofibrate	_
			8	p30s13_s	Clofibrate	_
			P	p30813_8	Ciolibrate	_ _
		Testing Set				
			No.	Sample	Label	_
			25 26	p30s10_s p30s15 s	Wyeth Wyeth	
			20	p30s15_s p30s27_s	Wyeth	
		Insert >>	28	p30s08_s	Clofibrate	
		<< Remove	29	p30s24_s	Clofibrate	
			30	p30s39_s	Clofibrate	
			31	p30s18_s	Gemfibrozil	
			32	p30s45_s	Gemfibrozil	
l				p		
		Submit				

9. Select a vigilance value from the slider

Expression Predictor						
iect						
Parameters Prediction						
ie: D:\Demo\Sample\FuzzyArtMapSample.txt						
e. D.Denio Sampley azzym wapsample. At						
alidation: Training/Testing Set Leave One Out Cross Validation 	Apply All Values	in Vigilance	Spectrum			
igilance:	5 0.6	0.7	0.8	0.9 1.0		
raining/Testing Set Selection						
Original Set	Training Set					
No. Sample Label			No.	Sample	Label	
,,		1		p30s11_s	Wyeth	
		2		p30s16_s	Wyeth	
	Insert >>	3		p30s28_s	Wyeth	
	mserter	4		p30s17_s	Wyeth	
	<< Remove	5		p30s29_s	Wyeth	
		6		p30s41_s	Wyeth	
		7		p30s09_s	Clofibrate	
		8		p30s13_s	Clofibrate	_
				- F -		
	Testing Set					
			No.	Sample	Label	
		25		p30s10_s	Wyeth	
		26		p30s15_s	Wyeth	
	Insert >>	27		p30s27_s	Wyeth	
	moert	28		p30s08_s	Clofibrate	
	<< Remove	29		p30s24_s	Clofibrate	
		30		p30s39_s	Clofibrate	
		31		p30s18_s	Gemfibrozil	
		32		p30s45_s	Gemfibrozil	-
	Submit					

10. Click on the "Submit" button

xpression Predictor							_
ect							
Provident I							
arameters Prediction							
: D:'Demo'Sample'FuzzyArtMapSample.txt							
: D:Demo Sample FuzzyArtMapSample.txt							
	_	_					
lidation: 🖲 Training/Testing Set 🛛 Leave One	Out Cross Validation	Apply All Values	s in Vigilanc	e Spectrun	1		
jilance: 0.0 0.1 0.2 0.3	0.4 0.5	0.6	0.7	0.8	0.9 1.0		
	0.4 0.3	0.0	0.7	0.0	0.9 1.0		
aining/Testing Set Selection							
Original Set		Training Set					
No. Sample	Label			No.	Sample	Label	
into. Oumpic	Editor		1	INU.	p30s11_s	Wyeth	
			2		p30s16_s	Wyeth	
		In contract	3		p30s28_s	Wyeth	
		Insert >>	4		p30s17_s	Wyeth	
		<< Remove	5		p30s29_s	Wyeth	
			6		p30s41_s	Wyeth	
			7		p30s09_s	Clofibrate	
			8		p30s13_s	Clofibrate	
			-		h		
		Testing Set					
				No.	Sample	Label	
			25		p30s10_s	Wyeth	
			26		p30s15_s	Wyeth	
		Insert >>	27		p30s27_s	Wyeth	
		msert	28		p30s08_s	Clofibrate	
		<< Remove	29		p30s24_s	Clofibrate	
			30		p30s39_s	Clofibrate	
			31		p30s18_s	Gemfibrozil	
			32		p30s45_s	Gemfibrozil	-
		Cutury?					
		Submit					

11. Click on the Prediction Tab to view the confusion matrix

Γ	Expression Predictor				_ 🗆 ×
F	Project				
Γ	Parameters Prediction				
L	Prediction	Clofibrate	Gemfibrozil	Phenobarbital	Wyeth
	Clofibrate	1	0	0	0
	Gemfibrozil	2	3	0	0
	Phenobarbital	0	0	3	0
	Wyeth	0	0	0	3
	No Prediction	0	0	0	0
		.33%. 3.67%.			

12. Click on one of the numbers in the confusion matrix to view the list of samples that corresponds the prediction in the selected cell from the matrix.

Expression Predictor				_ 🗆 ×
Project				
Parameters Prediction				
Prediction	Clofibrate	Gemfibrozil	Phenobarbita	
Clofibrate	1	0	0	0
Gemfibrozil	2	3	0	0
Phenobarbital	0	0	3	0
Wyeth No Prediction	0	0	0	3
-				
Statistical summary over 12 run -				
There is total 10 right prediction 83				
There is total 2 wrong prediction 16				
There is total 0 no prediction 0.00%				
🔮 Prediction: Clofib	rate			
No.	Sample	9	Label	1

No.	Sample	Label
28	p30s08_s	Clofibrate

1.2 Training/Testing Set Validation over the Entire Vigilance Spectrum

- 1. Repeat steps 1 to 8 from Section 1.1
- 2. Click on the checkbox that says "Apply All Values in Vigilance Spectrum"

rs Prediction PDemo'FuzzyArtMa	apSample.txt						
Training/Test	ting Set 🛛 Leave On	e Out Cross Validatior	n 🔽 Apply All Values i	n Vigilance Spectrur	n		
esting Set Selecti	ion						
al Set	011						
			Training Set				
No.	Sample	Label		No.	Sample	Label	
				1	p30s11_s	Wyeth	-
				2	p30s16_s	Wyeth	
			Insert >>	3	p30s28_s	Wyeth	
				4	p30s17_s	Wyeth	_
			<< Remove	5	p30s29_s	Wyeth	_
				6	p30s41_s	Wyeth	
				8	p30s09_s	Clofibrate Clofibrate	
				8	p30s13_s	Ciolibrate	-
			Testing Set				
				No.	Sample	Label	
				25	p30s10_s	Wyeth	-
				26	p30s15_s	Wyeth	
			Insert >>	27	p30s27_s	Wyeth	
			Maciter	28	p30s08_s	Clofibrate	
			<< Remove	29	p30s24_s	Clofibrate	
				31	p30s18_s	Gemfibrozil	
				32	p30s45_s	Gemfibrozil	-
			<< Remove	29 30	p30s24_s p30s39_s p30s18_s	Clofibrate Clofibrate Gemfibrozil	

- 3. Repeat steps 10 from Section 1.1
- 4. Click on Prediction Tab to view the prediction results using vigilance values from 0 to 1 with 0.01 increment at each cycle

Parameters Prediction				
Vigilance	Right Prediction(%)	Wrong Prediction(%)		No Prediction(%)
.00	91.67	8.33	0.00	
.01	91.67	8.33	0.00	
.02	91.67	8.33	0.00	
.03	91.67	8.33	0.00	
.04	91.67	8.33	0.00	
1.05	91.67	8.33	0.00	
1.06	91.67	8.33	0.00	
1.07	91.67	8.33	0.00	
1.08	91.67	8.33	0.00	
1.09	91.67	8.33	0.00	
.10	91.67	8.33	0.00	
l.11	91.67	8.33	0.00	
I.12	91.67	8.33	0.00	
l.13	91.67	8.33	0.00	
1.1.4	91.67	8.33	0.00	
1.15	91.67	8.33	0.00	
).16	91.67	8.33	0.00	
0.17	91.67	8.33	0.00	
).18	91.67	8.33	0.00	
).19	91.67	8.33	0.00	
0.20	91.67	8.33	0.00	
0.21	91.67	8.33	0.00	
0.22	91.67	8.33	0.00	
0.23	91.67	8.33	0.00	
0.24	91.67	8.33	0.00	
0.25	91.67	8.33	0.00	
.26	91.67	8.33	0.00	
0.27	91.67	8.33	0.00	
0.28	91.67	8.33	0.00	
0.29	91.67	8.33	0.00	
0.30	91.67	8.33	0.00	
1.31	91.67	8.33	0.00	
0.32	91.67	8.33	0.00	
0.33	91.67	8.33	0.00	
0.34	91.67	8.33	0.00	
.35	91.67	8.33	0.00	
1.36	91.67	8.33	0.00	
97	01.67	0.00	0.00	
				Save As Text (Tab delimited)

🍑 Save		×
Save in: 🔲	Demo 🗸	
FuzzyArtM	apSample.txt	
File <u>N</u> ame:	Prediction1.txt	
Files of <u>T</u> ype:	All Files	•
		Save Cancel

2.1 Leave One Out Cross Validation a Single Run

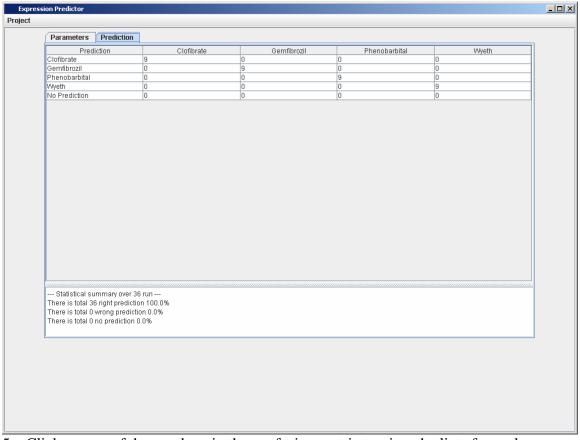
- Repeat steps 1 to 4 from Section 1.1
 Select Leave One Out Cross Validation

Expression Predictor	<u>- 🗆 ×</u>
Project	
Parameters Prediction	
File: D:'Demo'Sample/FuzzyArtMapSample.txt	
Validation: 🔘 Training/Testing Set 🔘 Leave One Out Cross Validation 🔲 Apply All Values in Vigilance Spectrum	
Vigilance: 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 Submit	

3. Click on the Submit button

Expression Predictor	_ 🗆 🗵
Project	
Parameters Prediction	
File: D:DemolSample/FuzzyArtMapSample.txt	
Validation: 🔾 Training/Testing Set 💿 Leave One Out Cross Validation 🗌 Apply All Values in Vigilance Spectrum	
Vigilance:	
Submit	

4. Click on the Prediction Tab to view the confusion matrix



5. Click on one of the numbers in the confusion matrix to view the list of samples that corresponds the prediction in the selected cell from the matrix.

Prediction Clofibrate Gemfibro2il Phenobarbital Wyeth Clofibrate 0	Chofitorate 9 0 0 0 Semfibrozil 0 9 0 0 0 Phenobarbital 0 0 9 0 0 Myeth 0 0 0 9 0		Prediction				
Semifibrozii 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Semifibrozii 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			Clofibrate			
Phenobarbital 0 0 0 0 9 0 0 9 0 0 9 0 0 0 9 0 0 0 0	Phenobarbital 0 0 0 0 9 0 0 9 0 0 9 0 0 0 9 0 0 0 0						
Wyeth 0 0 0 9 No Prediction 0 0 0 0	Wyeth 0 0 0 9 No Prediction 0 0 0 0						
No Prediction 0 0 0 0	No Prediction 0 0 0 0						
Statistical summary over 36 run Statistical summary over 36 run here is total 36 right prediction 100.0% here is total 0 wrong prediction 0.0%	Statistical summary over 36 run Statistical summary over 36 run here is total 36 right prediction 100.0% here is total 0 wrong prediction 0.0%						
Statistical summary over 36 run l'here is total 36 right prediction 100.0% l'here is total 0 wrong prediction 0.0%	Statistical summary over 36 run l'here is total 36 right prediction 100.0% l'here is total 0 wrong prediction 0.0%	vo Prediction	0		U	0	U
Statistical summary over 36 run There is total 36 right prediction 100.0% There is total 0 wrong prediction 0.0%	Statistical summary over 36 run There is total 36 right prediction 100.0% There is total 0 wrong prediction 0.0%						
There is total 36 right prediction 100.0% There is total 0 wrong prediction 0.0%	There is total 36 right prediction 100.0% There is total 0 wrong prediction 0.0%						
There is total 0 wrong prediction 0.0%	There is total 0 wrong prediction 0.0%						
There is total 0 wrong prediction 0.0% There is total 0 no prediction 0.0%		Statistical su	immary over 36 rur				
inere is total o no prediction o.o.%		Statistical su There is total 3	mmary over 36 rur 6 right prediction 11				
		Statistical su There is total 31 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			
		Statistical su There is total 3 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			
		Statistical su There is total 3 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			
		Statistical su There is total 3 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			
		Statistical su There is total 3 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			
		Statistical su There is total 3 There is total 0	mmary over 36 rur 6 right prediction 11 wrong prediction 0	.0%			

9 Prediction: Clo	fibrate	
No.	Sample	Label
7	p30s09_s	Clofibrate
8	p30s13_s	Clofibrate
9	p30s25_s	Clofibrate
10	p30s14_s	Clofibrate
11	p30s26_s	Clofibrate
12	p30s40_s	Clofibrate
28	p30s08_s	Clofibrate
29	p30s24_s	Clofibrate
30	p30s39_s	Clofibrate

2.2 Leave One Out Cross Validation over the Entire Vigilance Spectrum

- 1. Repeat steps 1 and 2 from Section 2.1
- 2. Click on the checkbox that says "Apply All Values in Vigilance Spectrum"

Expression Predictor	
Project	
Parameters Prediction	
File: D:Demo'Sample/FuzzyArtMapSample.txt	
Validation: 🔾 Training/Testing Set 💿 Leave One Out Cross Validation 📝 Apply All Values in Vigilance Spectrum	
Submit	
	_

3. Repeat steps 3 Section 2.1

4. Click on Prediction Tab to view the prediction results using vigilance values from 0 to 1 with 0.01 increment at each cycle

Parameters Prediction				
Vigilance	Right Prediction(%)	Wrong Prediction(%)	No Prediction(%)	Г
0.00	100.00	0.00	0.00	-
0.01	100.00	0.00	0.00	
D.02	100.00	0.00	0.00	
D.03	100.00	0.00	0.00	
D.04	100.00	0.00	0.00	
D.05	100.00	0.00	0.00	
D.06	100.00	0.00	0.00	
0.07	100.00	0.00	0.00	=
D.08	100.00	0.00	0.00	
D.09	100.00	0.00	0.00	
D.10	100.00	0.00	0.00	
D.11	100.00	0.00	0.00	
D.12	100.00	0.00	0.00	
D.13	100.00	0.00	0.00	
D.14	100.00	0.00	0.00	-17
D.15	100.00	0.00	0.00	11
D.16	100.00	0.00	0.00	11
D.17	100.00	0.00	0.00	-11
D.18	100.00	0.00	0.00	1
0.19	100.00	0.00	0.00	
0.20	100.00	0.00	0.00	1
D.21	100.00	0.00	0.00	1
0.22	100.00	0.00	0.00	-11
D.23	100.00	0.00	0.00	1
D.24 D.25	100.00	0.00	0.00	-17
	100.00	0.00	0.00	-17
0.26	100.00		0.00	-17
D.27 D.28	100.00	0.00	0.00	-
J.28 J.29	100.00	0.00		-
			0.00	-
D.30 D.31	100.00	0.00	0.00	-
J.31 J.32	100.00	0.00	0.00	-
J.32 J.33	100.00	0.00	0.00	-
J.33 J.34	100.00	0.00	0.00	
J.34 J.35	100.00	0.00	0.00	1
J.35 J.36	100.00	0.00	0.00	÷
1.30	100.00	0.00	0.00	•
			Save As Text (Tab delimited)	-

5. Repeat step 5 from Section 1.2 to save prediction as tab-delimited text file.