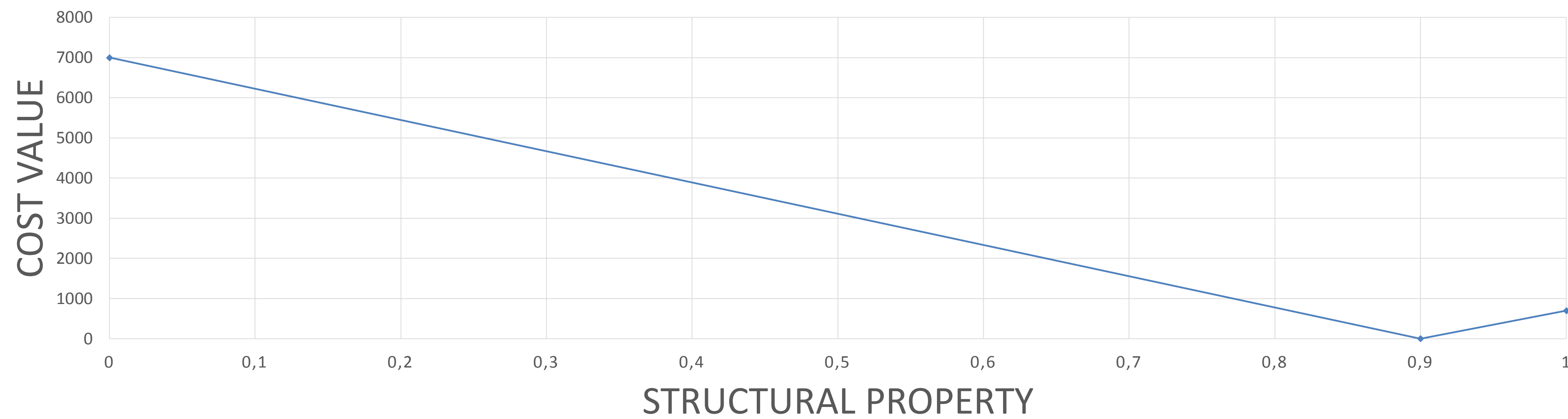


Graphlet-G4 cost function shape variability analysis

We investigate how the definition of the cost function influences the performance on a randomly reduced subset of 15 networks. The default penalty mapping is replaced by 15 different simple penalty mappings as shown below. All other parameters and penalty mappings were set to the default values. The AUPR scores are shown and compared to the scores obtained by using the default settings.

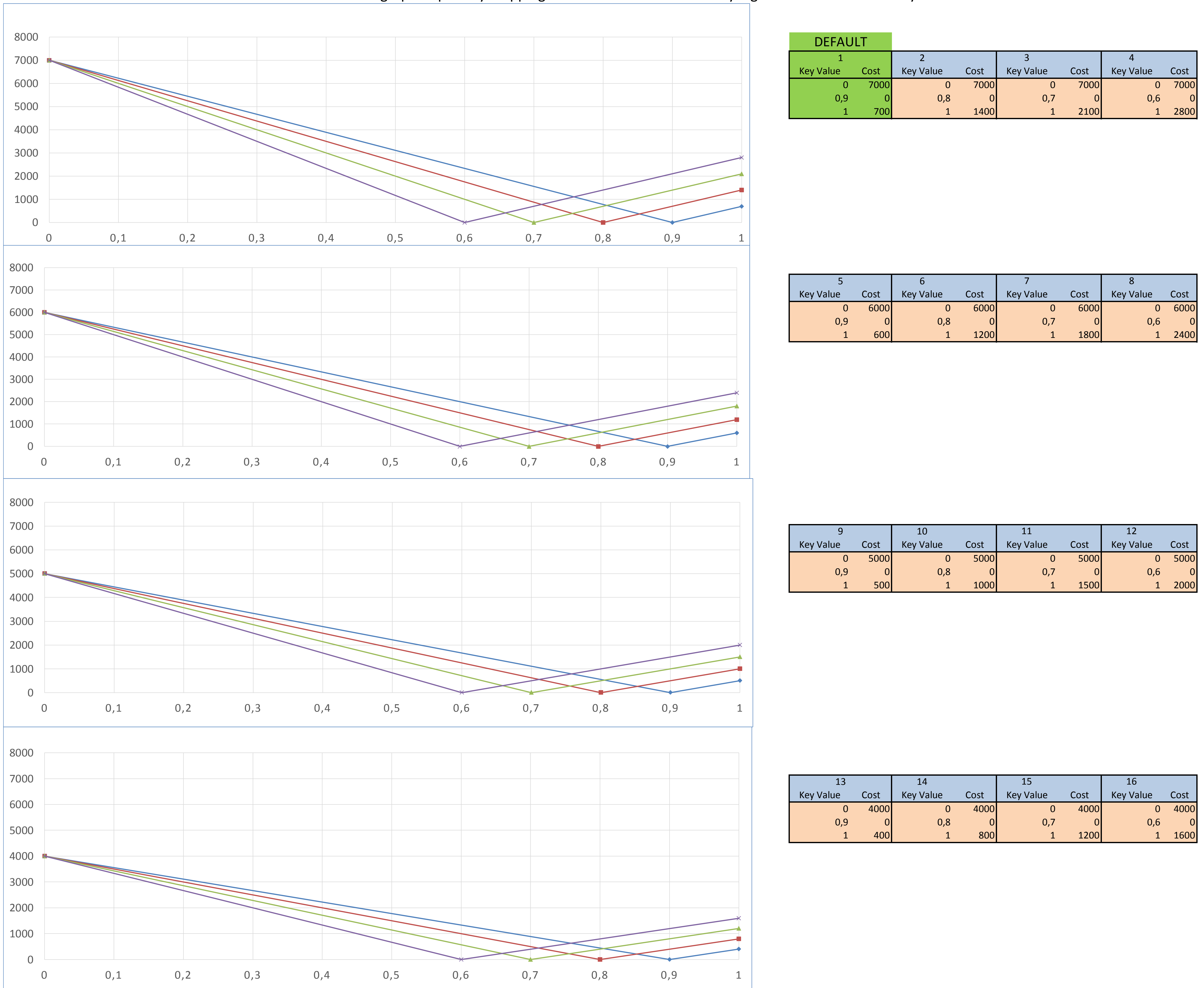
Default penalty function definition

G4-GRAPLET DEFAULT PENALTY MAPPING



Stability testing - Visualization of the grid search functions

We visualize the other G4-graphlet penalty mappings which were used in the 4 by 4 grid search in the stability tests.



Stability testing - Individual re-ranking AUPR scores

(1) Network inference algorithm used to obtain original prediction

(6) Difference in AUPR (altered - default)

Network	Original ranking	DEFAULT	GENIE3								GENIE3							
			1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
1 dream4-1	0.40	0.27	0.27	0.27	0.28	0.28	0.25	0.25	0.25	0.26	0.28	0.28	/	/	/	/	/	
2 dream4-3	0.49	0.51	0.51	0.51	0.52	0.53	0.49	0.51	0.51	0.52	0.52	0.52	/	/	/	/	/	
3 dream4-4	0.45	0.46	0.46	0.46	0.48	0.48	0.44	0.44	0.44	0.46	0.47	0.47	/	/	/	/	/	
4 dream5-1	0.94	0.94	0.94	0.88	0.87	0.87	0.94	0.89	0.86	0.87	0.87	0.87	/	/	/	/	/	
5 dream5-2	0.15	0.25	0.25	0.26	0.32	0.32	0.22	0.27	0.33	0.33	0.33	0.33	/	/	/	/	/	
6 gnw-200-1	0.37	0.72	0.72	0.71	0.71	0.71	0.72	0.71	0.71	0.71	0.71	0.71	/	/	/	/	/	
7 gnw-200-2	0.44	0.83	0.83	0.82	0.82	0.81	0.82	0.83	0.82	0.80	0.80	0.80	/	/	/	/	/	
8 gnw-200-5	0.27	0.33	0.33	0.33	0.33	0.33	0.33	0.32	0.33	0.31	0.31	0.31	/	/	/	/	/	
9 gnw-200-6	0.27	0.30	0.30	0.27	0.28	0.33	0.28	0.32	0.28	0.32	0.28	0.28	/	/	/	/	/	
10 gnw-200-7	0.30	0.41	0.41	0.42	0.41	0.42	0.43	0.43	0.43	0.41	0.41	0.41	/	/	/	/	/	
11 syntren-100-3	0.19	0.16	0.16	0.16	0.16	0.16	0.17	0.16	0.16	0.16	0.16	0.16	/	/	/	/	/	
12 syntren-100-4	0.17	0.17	0.17	0.17	0.17	0.17	0.18	0.17	0.17	0.17	0.17	0.17	/	/	/	/	/	
13 syntren-150-1	0.20	0.23	0.23	0.23	0.21	0.21	0.21	0.24	0.23	0.21	0.21	0.21	/	/	/	/	/	
14 syntren-150-3	0.30	0.41	0.41	0.41	0.42	0.42	0.43	0.44	0.40	0.40	0.40	0.40	/	/	/	/	/	
15 syntren-150-5	0.23	0.20	0.20	0.21	0.22	0.21	0.21	0.21	0.21	0.21	0.21	0.21	/	/	/	/	/	
Average All 15-networks	0.34	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	/	/	/	/	/	

(5) AUPR obtained by re-ranking with the altered penalty function (1,2,...,16) where the number corresponds to the plotted functions found above.

(4) AUPR obtained by re-ranking with Netter using the default parameters and penalty function

(3) AUPR score of the original prediction before re-ranking

(2) Network name (e.g. gnw-200-5 = network #5 in the GNW-200 dataset, each row is one network)

The table below lists the AUPR evaluation of the original prediction, the re-ranked prediction using default settings and all re-rankings obtained by using one of the altered penalty mappings found above. Each row is a network, each column is a re-ranking using a different setting.

Network	Original ranking	DEFAULT	GENIE3															
			1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00
1 dream4-1	0.40	0.27	0.27	0.27	0.28	0.28	0.25	0.25	0.25	0.26	0.28	0.28	/	/	/	/	/	
2 dream4-3	0.49	0.51	0.51	0.51	0.52	0.53	0.49	0.51	0.51	0.52	0.52	0.52	/	/	/	/	/	
3 dream4-4	0.45	0.46	0.46	0.46	0.48	0.48	0.44	0.44	0.44	0.46	0.47	0.47	/	/	/	/	/	
4 dream5-1	0.94	0.94	0.94	0.88	0.87	0.87	0.94	0.89	0.86	0.87	0.87	0.87	/	/	/	/	/	
5 dream5-2	0.15	0.25	0.25	0.26	0.32	0.32	0.22	0.27	0.33	0.33	0.33	0.33	/	/	/	/	/	
6 gnw-200-1	0.37	0.72	0.72	0.71	0.71	0.71	0.72	0.71	0.71	0.71	0.71	0.71	/	/	/	/	/	
7 gnw-200-2	0.44	0.83	0.83	0.82	0.82	0.81	0.82	0.83	0.82	0.80	0.80	0.80	/	/	/	/	/	
8 gnw-200-5	0.27	0.33	0.33	0.33	0.33	0.33	0.33	0.32	0.33	0.31	0.31	0.31	/	/	/	/	/	
9 gnw-200-6	0.27	0.30	0.30	0.27	0.28	0.33	0.28	0.32	0.28	0.32	0.28	0.28	/	/	/	/	/	
10 gnw-200-7	0.30	0.41	0.41	0.42	0.41	0.42	0.43	0.43	0.43	0.41	0.41	0.41	/	/	/	/	/	
11 syntren-100-3	0.19	0.16	0.16	0.16	0.16	0.16	0.17	0.16	0.16	0.16	0.16	0.16	/	/	/	/	/	
12 syntren-100-4	0.17	0.17	0.17	0.17	0.17	0.17	0.18	0.17	0.17	0.17	0.17	0.17	/	/	/	/	/	
13 syntren-150-1	0.20	0.23	0.23	0.23	0.21	0.21	0.21	0.24	0.23	0.21	0.21	0.21	/	/	/	/	/	
14 syntren-150-3	0.30	0.41	0.41	0.41	0.42	0.42	0.43	0.44	0.40	0.40	0.40	0.40	/	/	/	/	/	
15 syntren-150-5	0.23	0.20	0.20	0.21	0.22	0.21	0.21	0.21	0.21	0.21	0.21	0.21	/	/	/	/	/	
Average All 15-networks	0.34	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	/	/	/	/	/	

Network	Original ranking	DEFAULT	GENIE3															
			9.00	10.00	11.00	12.00	13.00	14.00	15.00	16.00	9.00	10.00	11.00	12.00	13.00	14.00	15.00	16.00
1 dream4-1	0.40	0.27	0.24	0.24	0.26	0.27	0.26	0.26	0.25	0.23	0.27	-0.03	-0.03	-0.01	0.00	0.00	0.00	
2 dream4-3	0.49	0.51	0.51	0.51	0.52	0.52	0.52	0.49	0.50	0.49	0.49	0.00	0.00	0.01	0.01	0.01	-0.02	
3 dream4-4	0.45	0.46	0.47	0.46	0.46	0.46	0.47	0.45	0.44	0.48	0.48	0.00	0.00	0.00	0.00	-0.01	-0.02	
4 dream5-1	0.94	0.94	0.95	0.88	0.87	0.87	0.94	0.89	0.88	0.88	0.88	0.01	-0.06	-0.06	-0.07	-0.05	-0.06	
5 dream5-2	0.15	0.25	0.23	0.26	0.34	0.33	0.22	0.25	0.34	0.33	0.33	-0.02	0.02	0.09	0.09	-0.02	0.00	
6 gnw-200-1	0.37	0.72	0.70	0.72	0.72	0.72	0.72	0.71	0.71	0.69	0.69	-0.01	-0.01	0.00	0.00	0.01	0.00	
7 gnw-200-2	0.44	0.83	0.83	0.82	0.82	0.82	0.83	0.83	0.82	0.81	0.81	-0.01	-0.01	0.01	-0.01	0.00	0.01	
8 gnw-200-5	0.27	0.33	0.32	0.32	0.32	0.32	0.33	0.33	0.33	0.31	0.31	-0.01	-0.01	0.00	-0.01	0.00	0.01	
9 gnw-200-6	0.27	0.30	0.28	0.27	0.26	0.32	0.27	0.26	0.27	0.28	0.28	-0.01	-0.03	-0.03	-0.02	-0.02	-0.02	
10 gnw-200-7	0.30	0.41	0.43	0.43	0.42	0.40	0.42	0.42	0.43	0.41	0.41	0.02	0.02	0.00	-0.01	0.00	0.01	
11 syntren-100-3	0.19	0.16	0.16	0.17	0.16	0.16	0.16	0.17	0.17	0.17	0.17	0.00	0.01	0.00	0.00	0.00	0.01	
12 syntren-100-4	0.17	0.17	0.18	0.17	0.17	0.17	0.17	0.18	0.18	0.17	0.17	0.01	0.00	0.00	0.00	0.01	0.01	
13 syntren-150-1	0.20	0.23	0.26	0.23	0.23	0.22	0.22	0.26	0.24	0.24	0.24	0.03	0.00	0.00	-0.01	-0.01	0.03	
14 syntren-150-3	0.30	0.41	0.44	0.45	0.43	0.43	0.43	0.43	0.45	0.42	0.42	0.02	0.04	0.02	0.02	0.02	0.04	
15 syntren-150-5	0.23	0.20	0.20	0.20	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.00	0.00	0.01	0.00	0.00	0.01	
Average All 15-networks	0.34	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.00	0.00	0.00	0.00	0.00	0.00	

Stability testing - Varying the relative weighing parameter variability analysis

We investigate what the effect is of making the penalty more or less important in the total cost function. This is done by varying the coefficient on a randomly reduced subset of 15 networks. AUPR values are shown.

(1) Network inference algorithm used to obtain original prediction

(6) Difference in AUPR (altered -default)

Network	Original ranking	DEF, = 75	GENIE3							
			/	1	5	10	Δ/	Δ1	Δ5	Δ10
1 dream4-1	0.40	0.28	0.31	0.25	0.32	0.39	0.03	-0.04	0.03	0.11
2 dream4-3	0.49	0.52	0.50	0.48	0.52	0.50	-0.02	-0.05	0.00	-0.02
3 dream4-4	0.45	0.46	0.49	0.49	0.50	0.51	-0.01	-0.01	0.00	0.00
4 dream5-1	0.94	0.94	0.94	0.94	0.94	0.95	0.00	0.00	0.00	0.00
5 dream5-2	0.15	0.25	0.27	0.25	0.26	0.23	0.01	0.00	0.01	-0.03
6 gnw-200-1	0.37	0.68	0.56	0.68	0.68	0.68	-0.12	0.01	0.00	0.00
7 gnw-200-2	0.44	0.76	0.54	0.75	0.77	0.81	-0.22	-0.02	0.00	0.04
8 gnw-200-5	0.27	0.35	0.30	0.34	0.34	0.32	-0.04	0.00	-0.01	-0.02
9 gnw-200-6	0.27	0.35	0.28	0.34	0.36	0.36	-0.07	-0.01	0.01	0.01
10 gnw-200-7	0.30	0.42	0.44	0.46	0.41	0.40	0.02	0.03	-0.02	-0.03
11 syntren-100-3	0.19	0.16	0.15	0.17	0.16	0.16	-0.01	0.01	0.00	0.00
12 syntren-100-4	0.17	0.16	0.17	0.18	0.18	0.17	0.01	0.01	0.01	0.00
13 syntren-150-1	0.20	0.24	0.23	0.22	0.21	0.20	-0.02	-0.02	-0.04	-0.05
14 syntren-150-3	0.30	0.39	0.41	0.40	0.37	0.36	0.02	0.02	-0.02	-0.03
15 syntren-150-5	0.23	0.21	0.20	0.21	0.21	0.21	-0.01	0.00	0.01	0.00
Average All 15-networks	0.34	0.42	0.39	0.41	0.41	0.42	-0.03	-0.01	0.00	0.00

(5) AUPR using a different relative weigh. coef.

(4) AUPR score obtained using default settings and penalties

(3) AUPR initial prediction (before re-ranking)

(2) Network name, each row is a network

Network	Original ranking	DEF, = 75	GENIE3									
			/	1	5	10	Δ/	Δ1	Δ5	Δ10		
1 dream4-1	0.40	0.28	0.31	0.25	0.32	0.39	0.03	-0.04	0.03	0.11		
2 dream4-3	0.49	0.52	0.50	0.48	0.52	0.50	-0.02	-0.05	0.00	-0.02		
3 dream4-4	0.45	0.51	0.49	0.49	0.50	0.51	-0.01	-0.01	0.00	0.00		
4 dream5-1	0.94	0.94	0.94	0.94	0.94	0.95	0.00	0.00	0.00	0.00		
5 dream5-2	0.15	0.25	0.27	0.25	0.26	0.23	0.01	0.00	0.01	-0.03		
6 gnw-200-1	0.37	0.68	0.56	0.68	0.68	0.68	-0.12	0.01	0.00	0.00		
7 gnw-200-2	0.44	0.76	0.54	0.75	0.77	0.81	-0.22	-0.02	0.00	0.04		
8 gnw-200-5	0.27	0.35	0.30	0.34	0.34	0.32	-0.04	0.00	-0.01	-0.02		
9 gnw-200-6	0.27	0.35	0.28	0.34	0.36	0.36	-0.07	-0.01	0.01	0.01		
10 gnw-200-7	0.30	0.42	0.44	0.46	0.41	0.40	0.02	0.03</				