Results of Challenge 1

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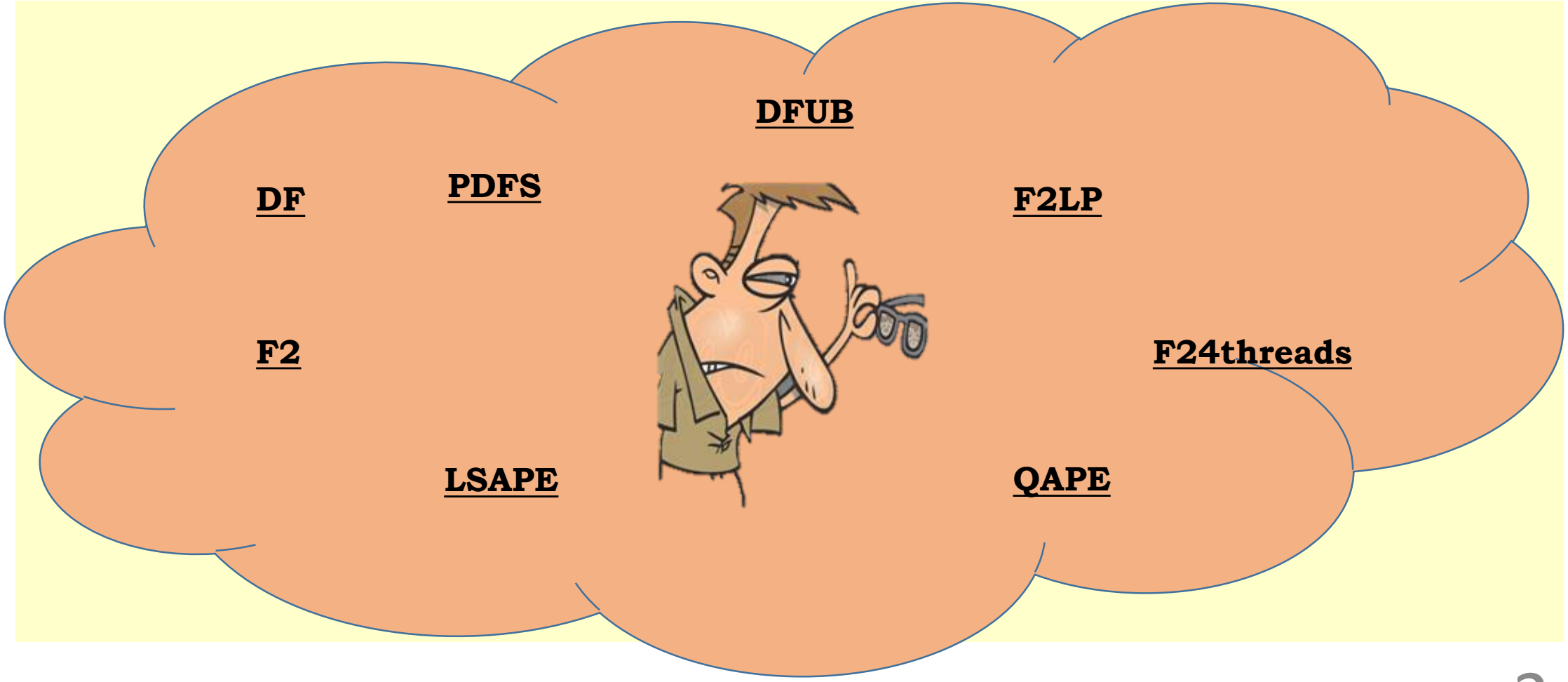
Inspection



Outline

- Datasets and Protocol
- Results
- Conclusion
- Perspectives

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Characterstics of Datasets

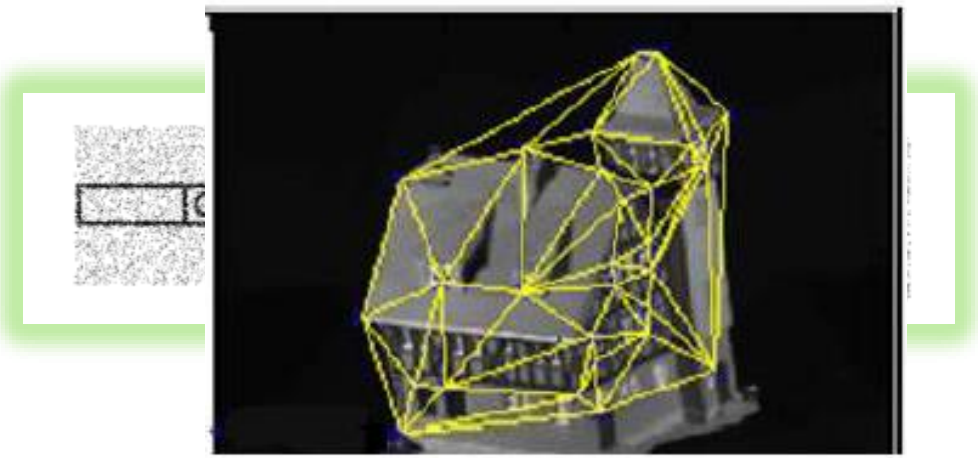
Symbolic

Dataset	# graphs	Max # nodes	Max # edges	Avg(Vertices)	Avg(Edges)	Avg Density	Vertix attributes	Edge Attributes
MUTA	4337	417	112	30.317	30.769	2.029	Chemical symbol	Valence
Acyclic	185	11	10	8.146	7.146	1.755	Chemical symbol	Valence
Alkane	150	10	9	8.873	7.873	1.774	Chemical symbol	Valence
MAO	68	27	29	18.382	19.632	2.136	Chemical symbol	Valence
PAH	94	28	34	20.702	24.425	2.359	Chemical symbol	Valence

Characteristics of Datasets

Numeric

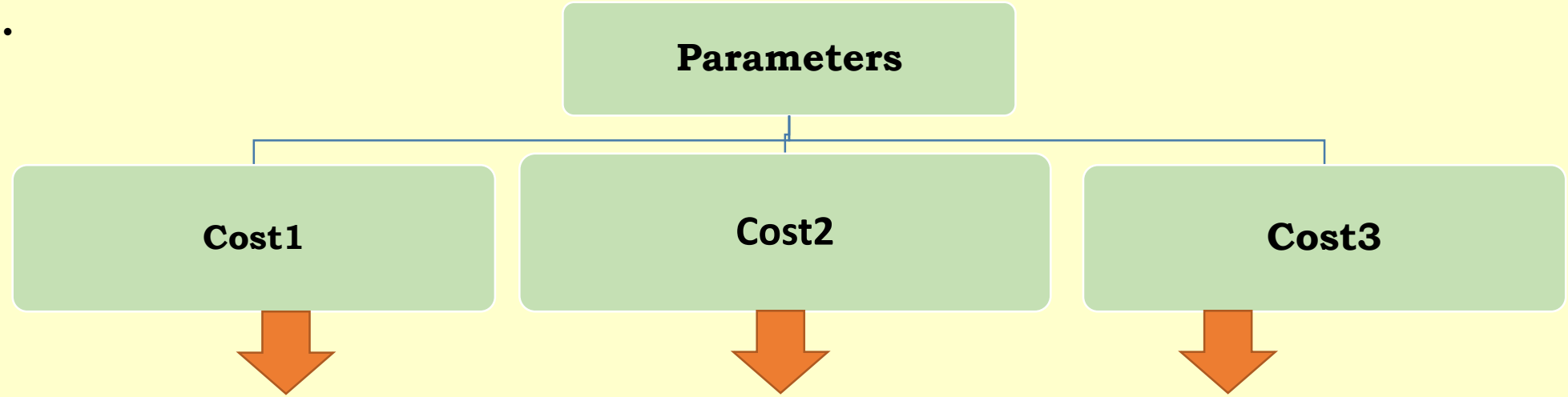
Dataset	# graphs	Max # nodes	Max # edges	Avg(Vertices)	Avg(Edges)	Avg Density	Vertix attributes	Edge Attributes
GREC	1100	24	29	11.509	11.934	2.073	x,y coordinates	Line type
CMU	111	30	80	30	79.108	5.274	None	Distance between points



Datasets for Scalability

	# Datasets	# Graphs	# Vetices	Vertex Attributes	Edge Attributes	Exact GED
MUTA	7	10	10			NO
			20			
			30			
			40			
			50			
			60			
			70			
			MIX			
GREC	5	10	5			YES
			10			
			15			
			20			
			MIX			

Protocol: Symbolic Datasets



Insertion/deletion (nodes)= 4
Node substitutions = 2
Edge substitutions/deletions/insertions = 1

Insertion/deletion (nodes)= 4
Node substitutions = 2
Edge deletions and insertions = 2
Edge substituions = 1

Insertion/deletion (nodes)= 2
Node substitutions = 6
Edge deletions and insertions = 1
Edge substituions = 3

Protocol: Constraints

- **For parallel algorithms:**
  - Number of threads = 4
- **Time constraint:** 30 seconds per comparision

Protocol: Metrics

1. **Deviation:**

$$dev(g_i, g_j)^p = \frac{|d(g_i, g_j)^p - R_{g_i,g_j}|}{R_{g_i,g_j}}, \forall (i,j) \in [\![1, m]\!]^2, \forall p \in \mathcal{P} \qquad (1)$$

2. **Number of Optimal Solutions:**
   - Before timing out (with and without optimality proof)

3. **Execution Time**
   - In seconds

Protocol: Metrics

4. Deviation - Time

$$\overline{dev^p} = \frac{1}{m \times m} \sum_{i=1}^{m} \sum_{j=1}^{m} dev(g_i, g_j)^p$$

$$\overline{deviation\_score^p} = \frac{1}{\#subsets} \sum_{i=1}^{\#subsets} \frac{\overline{dev_i^p}}{max\_dev_i}$$

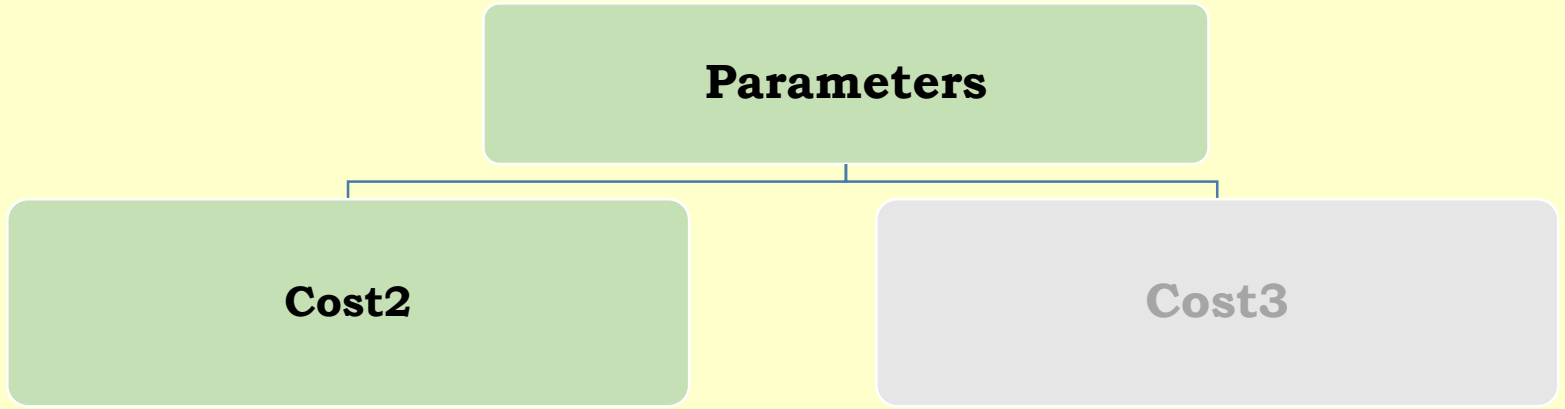
$$\overline{time^p} = \frac{1}{m \times m} \sum_{i=1}^{m} \sum_{j=1}^{m} time(g_i, g_j)^p \; and \; (i,j) \in [\![1, m]\!]^2$$

$$\overline{time\_score^p} = \frac{1}{\#subsets} \sum_{i=1}^{\#subsets} \frac{\overline{time_i^p}}{max\_time_i}$$

Outline

- Reminder
- Results
  - Symbolic Databases
    - Mutagenicity
    - Acyclic, Alkane and Mao
  - Numeric Databases
    - GREC
    - CMU
- Conclusion
- Perspectives

Mutagenicity



Insertion/deletion (nodes)= 4

Node substitutions = 2

Edge deletions and insertions = 2

Edge substituions = 1

Mutagenicity – COST2 - Deviation

	Assignment Problem Based methods			Binary linear programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
MUTA-10	13.769	54.456	11.270	**0**	**0**	15.186	**0**	28.554	**0**
MUTA-20	49.054	86.870	25.971	0.547	**0**	47.308	42.278	64.687	25.716
MUTA-30	48.628	91.132	27.498	11.179	**1.369**	72.450	47.624	66.615	37.903
MUTA-40	59.997	89.868	22.670	18.591	**1.842**	65.052	58.678	71.280	50.340
MUTA-50	55.078	84.990	**5.214**	26.893	**6.539**	46.954	57.334	70.072	47.937
MUTA-60	45.563	88.332	**3.335**	43.395	11.144	47.900	48.201	65.286	38.746
MUTA-70	69.847	86.487	**2.490**	56.530	26.961	57.691	42.855	57	36.300
MUTA-MIX	26.347	45.623	3.719	9.375	**1.802**	18.559	25.721	30.948	22.442

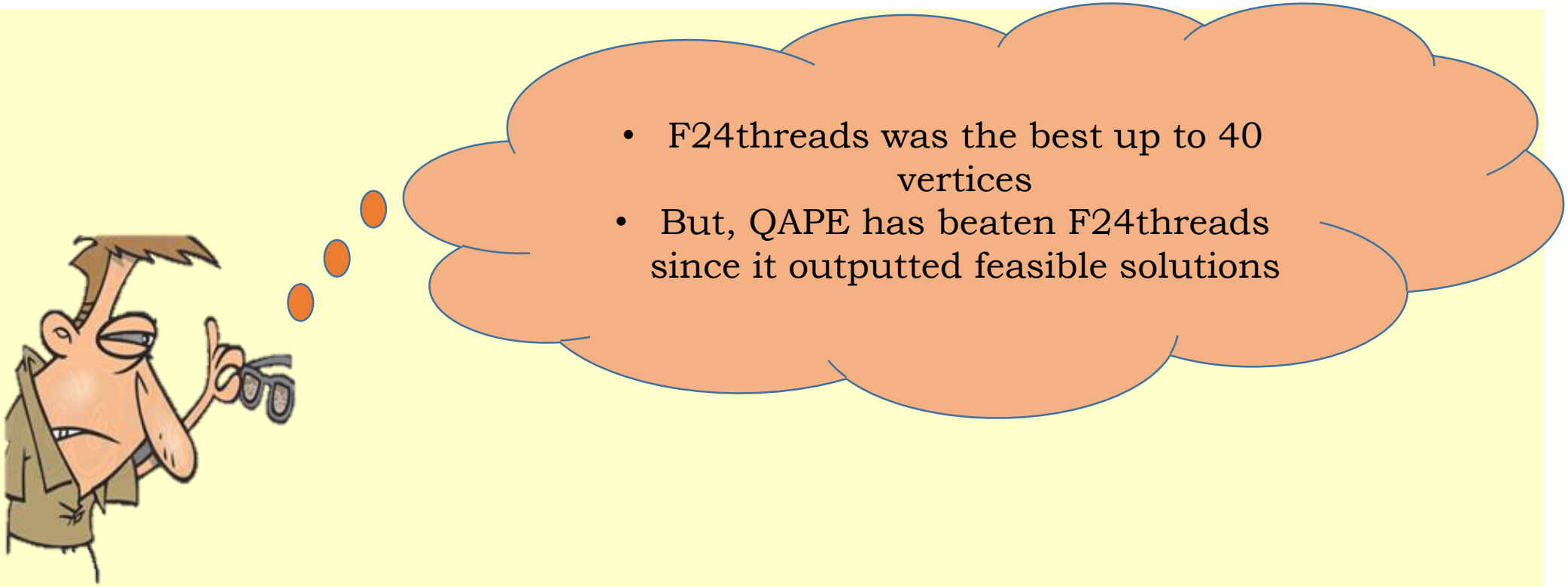
Mutagenicity – COST2 - % Proved/Unproved Optimal Soltuion

	Assignment Problem Based methods			Binary linear programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
MUTA-10	42	20	50	**100**	**100**	46	**100**	28	**100**
MUTA-20	10	10	13	94	**98**	16	14	10	26
MUTA-30	10	8	10	15	**23**	10	10	10	11
MUTA-40	10	10	10	11	**12**	9	10	10	10
MUTA-50	10	10	10	10	**10**	10	10	10	10
MUTA-60	10	9	10	10	**10**	9	10	10	10
MUTA-70	10	10	10	10	**10**	9	10	10	10
MUTA-MIX	10	9	14	41	**44**	10	11	10	13

Mutagenicity – COST2 – Running Time

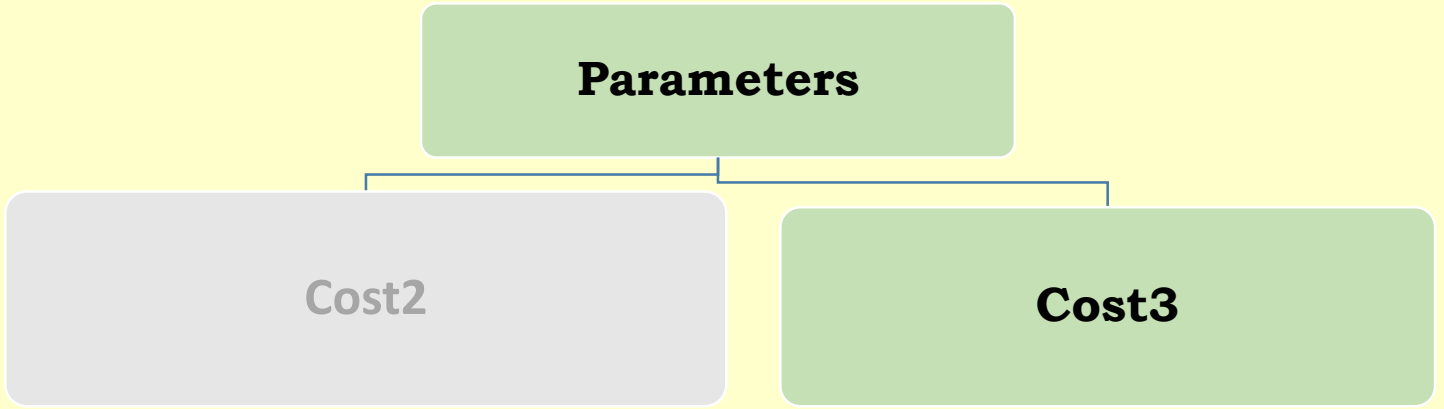
	Assignment Problem Based methods			Binary linear programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
MUTA-10	0.155	0.025	**0.037**	0.608	0.606	0.575	1.703	**0.037**	1.239
MUTA-20	0.558	0.108	0.166	6.243	3.574	1.380	27.052	**0.088**	26.651
MUTA-30	1.541	0.458	0.495	25.724	24.701	3.091	27.080	**0.142**	27.081
MUTA-40	3.416	1.475	1.405	27.500	27.392	7.697	27.098	**0.217**	27.100
MUTA-50	7.213	4.253	4.337	30.006	29.916	16.511	27.172	**0.287**	27.173
MUTA-60	14.945	11.694	11.551	34.147	34.134	30.360	27.230	**0.369**	27.232
MUTA-70	28.423	27.764	27.092	42.202	42.101	42.085	27.372	**0.498**	27.375
MUTA-MIX	11.690	4.986	4.920	22.892	21.512	14.148	27.173	**0.268**	26.964

Conclusion 1



- F24threads was the best up to 40 vertices
- But, QAPE has beaten F24threads since it outputted feasible solutions

Mutagenicity



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Mutagenicity – COST3 - Deviation

		Assignment Problem Based methods		Binary Linear Programming Based Approaches			Branch-and-Bound based Approaches		
	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
MUTA-10	4.027	22.623	4.073	**0**	**0**	1.675	**0**	16.321	**0**
MUTA-20	15.954	40.025	4.043	**0**	**0**	7.267	16.798	30.280	9.581
MUTA-30	29.123	70.803	15.009	1.195	**0.431**	26.050	27.222	39.243	24.991
MUTA-40	36.629	74.005	13.986	3.183	**0.212**	15.864	39.934	47.710	33.918
MUTA-50	47.073	75.775	10.198	4.220	**0.309**	12.809	50.943	60.497	45.818
MUTA-60	37.009	81.610	7.793	8.893	**0.634**	13.588	41.268	49.442	36.695
MUTA-70	79.810	77.971	7.809	12.566	**0.158**	14.101	37.079	46.373	34.034
MUTA-MIX	20.437	39.308	3.662	2.531	**0.244**	7.393	20.101	26.542	16.699

Mutagenicity – COST3 - % Proved/Unproved Optimal Solutions

		Assignment Problem based methods		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
MUTA-10	65	23	74	**100**	**100**	77	100	25	100
MUTA-20	14	10	47	**100**	**100**	40	14	10	26
MUTA-30	10	3	14	57	**66**	15	11	10	12
MUTA-40	10	4	11	31	**41**	12	10	10	10
MUTA-50	10	5	11	18	**23**	11	10	10	10
MUTA-60	10	3	10	10	**11**	10	10	10	10
MUTA-70	10	2	10	12	**12**	10	10	10	10
MUTA-MIX	13	5	24	55	**58**	21	14	10	20

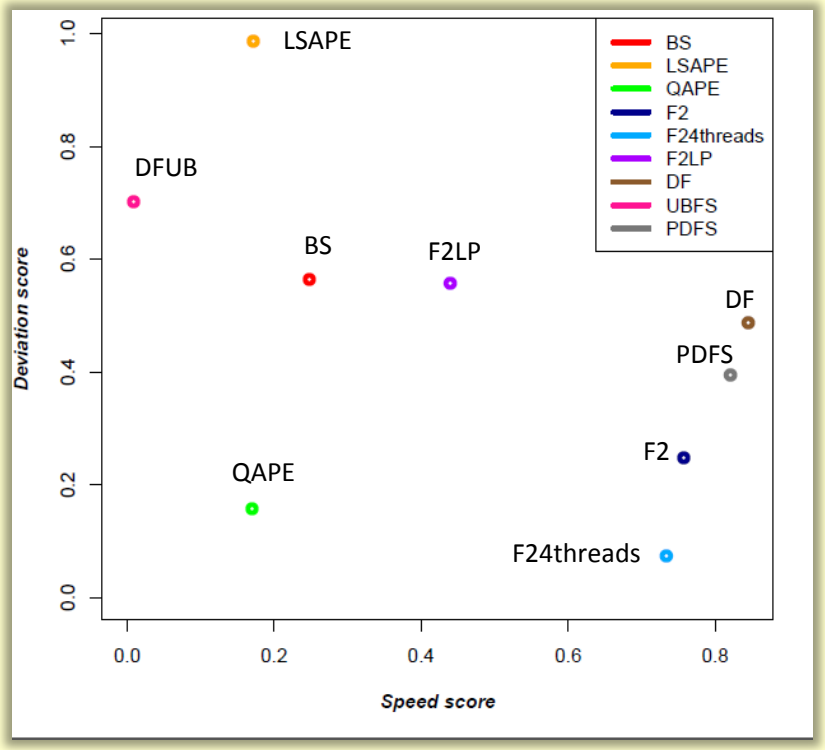
Mutagenicity – COST3 – Running Time

	Assignment Problem Based methods		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
MUTA-10	0.165	**0.018**	0.037	0.479	0.490	0.462	1.345	0.038	0.943
MUTA-20	0.600	0.109	0.161	1.694	1.306	1.089	26.724	**0.092**	26.563
MUTA-30	1.625	0.443	0.521	18.407	14.480	2.593	27.090	**0.147**	27.082
MUTA-40	3.625	1.367	1.433	25.300	23.280	6.294	27.098	**0.221**	27.101
MUTA-50	7.632	4.229	4.357	29.454	28.562	13.083	27.169	**0.293**	27.172
MUTA-60	15.573	11.543	11.597	34.061	33.979	23.501	27.230	**0.373**	27.234
MUTA-70	28.557	27.800	**27.439**	41.699	41.724	39.938	27.354	**0.495**	27.358
MUTA-MIX	11.506	4.944	4.972	19.600	18.350	11.257	26.462	**0.274**	25.430

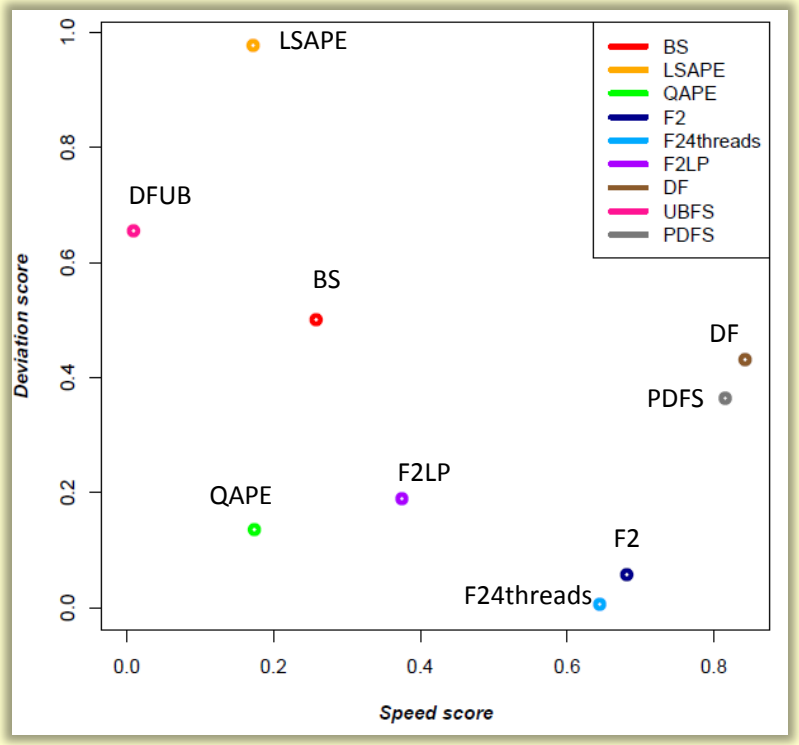
Conclusion 2

F24threads was always the best … it seems there was a big influence of COST3

To sum up: Time-Deviation Scores



Cost 2



Cost 3

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Symbolic Datasets - Deviation

Acyclic

		Assignment Problem Based methods		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	21.682	38.437	9.390	**0**	**0**	14.813	0.045	33.796	0.007
COST2	34.016	55.823	13.732	**0**	**0**	25.266	0.080	45.938	0.019
COST3	22.304	40.136	10.141	**0**	**0**	11.825	0.056	36.059	0.017

Alkane

	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	16.623	65.654	18.939	**0**	**0**	38.507	**0**	19.776	**0**
COST2	20	75.340	23.264	**0**	**0**	46.632	**0**	23.928	**0**
COST3	18.258	73.766	21.482	**0**	**0**	44.728	**0**	21.979	**0**

Symbolic Datasets - Deviation

Mao

	Assignment Problem Based methods			Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	5.980	30.953	2.017	**0**	**0**	1.242	0.349	11.254	1.589
COST2	9.427	45.677	2.779	**0**	**0**	**0**	0.763	16.157	2.784
COST3	7.880	76.581	5.921	**0**	**0**	2.330	0.877	13.902	2.001

PAH

	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	49.484	93.919	41.361	13.541	**1.294**	92.706	33.827	56.308	31.023
COST2	62.790	98.665	54.656	17.882	**3.278**	65.105	45.019	70.246	41.550
COST3	59.830	97.237	51.627	15.315	**1.426**	96.530	42.137	67.414	38.656

Acyclic – % Optimal Solutions

		Assignment Problem Based methods			Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
		BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
Proved to be optimal	**COST1**	0	0	0	**100**	**100**	48.636	97.255	0	99.059
	COST2	0	0	0	**100**	**100**	30.499	96.488	0	98.542
	COST3	0	0	0	**100**	**100**	50.431	95.207	0	97.790
		BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
Proved or unproved to be optimal	COST1	19.394	9.677	64.340	**100**	**100**	56.484	99.782	8.764	99.967
	COST2	13.464	7.865	57.165	**100**	**100**	42.575	99.647	7.402	99.922
	COST3	20.042	10.283	57.759	**100**	**100**	58.156	99.674	9.280	99.895

Alkane – % Optimal Solutions

Assignment Problem Based methods | Binary Linear Programming based Approaches | Branch-and-Bound based Approaches

Proved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	0	0	0	**100**	**100**	21.937	**100**	0	**100**
COST2	0	0	0	**100**	**100**	22.048	**100**	0	**100**
COST3	0	0	0	**100**	**100**	22.048	**100**	0	**100**

Proved or unproved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	59.448	5.431	54.715	**100**	**100**	29.746	99.613	52.546	**100**
COST2	59.835	5.817	54.546	**100**	**100**	29.933	100	52.933	**100**
COST3	59.835	5.817	54.546	**100**	**100**	29.928	100	52.933	**100**

MAO – % Optimal Solutions

Assignment Problem Based methods | Binary Linear Programming based Approaches | Branch-and-Bound based Approaches

Proved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	0	0	0	**100**	**100**	83.564	81.725	0	80.774
COST2	0	0	0	**100**	**100**	**100**	75.324	0	76.384
COST3	0	0	0	**100**	**100**	93.209	85.964	0	85.488

Proved or unproved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	72.577	19.355	77.573	**100**	**100**	89.100	98.421	56.444	95.436
COST2	67.236	16.976	79.044	**100**	**100**	**100**	97.945	56.293	94.442
COST3	74.372	1.384	72.534	**100**	**100**	86.029	96.799	59.580	94.809

PAH – % Optimal Solutions

Assignment Problem Based methods | Binary Linear Programming based Approaches | Branch-and-Bound based Approaches

Proved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	0	0	0	57.729	83.918	0.724	12.052	0	15.799
COST2	0	0	0	58.125	83.431	0.837	12.052	0	15.821
COST3	0	0	0	58.465	83.918	0.837	12.030	0	15.844

Proved or unproved to be optimal

	BS	LSAPE	QAPE	F2	F24threads	F2LP	DF	DFUB	PDFS
COST1	4.741	1.063	9.042	61.736	84.019	0.882	16.772	3.225	20.348
COST2	4.538	1.063	9.325	61.407	83.080	2.206	16.455	3.066	20.133
COST3	4.730	1.063	9.574	62.426	83.997	1.063	16.862	3.225	20.484

Symbolic Datasets – Running Time

Acyclic

		Assignment Problem Based methods		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	**0.127**	**0.010**	**0.024**	0.792	0.839	0.781	2.949	**0.036**	1.976
COST2	**0.127**	**0.010**	**0.023**	0.815	0.865	0.788	3.351	**0.036**	2.359
COST3	**0.128**	**0.010**	**0.024**	0.790	0.837	0.780	4.320	**0.036**	2.967

Alkane

	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	**0.133**	**0.013**	**0.029**	0.833	0.918	0.809	0.705	**0.035**	0.517
COST2	**0.133**	**0.014**	**0.028**	0.835	0.931	0.808	0.706	**0.035**	0.493
COST3	**0.201**	**0.014**	**0.028**	0.835	0.922	0.808	0.703	**0.035**	0.526

Symbolic Datasets – Running Time

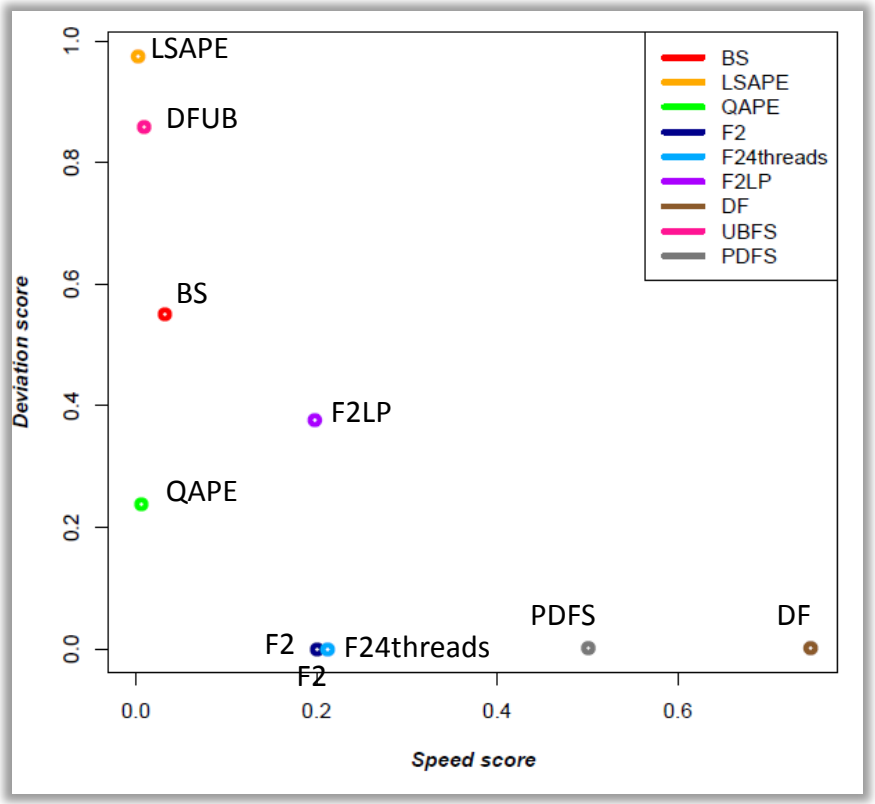
Mao

		Assignment Problem Based methods		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	**0.559**	**0.097**	**0.128**	1.065	1.047	1.050	6.996	0.083	7.368
COST2	**0.562**	**0.094**	**0.123**	1.268	1.513	1.268	8.858	0.083	8.806
COST3	**0.537**	**0.086**	**0.126**	0.979	0.990	0.977	5.513	0.083	5.793

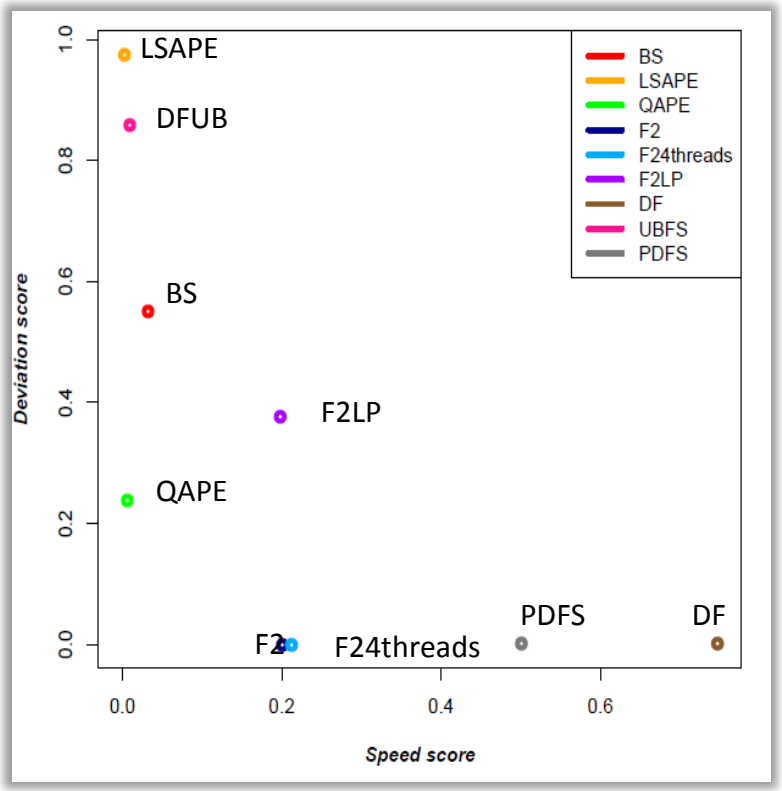
PAH

	BS	**LSAPE**	**QAPE**	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
COST1	**0.786**	**0.141**	**0.196**	18.782	11.428	2.709	27.446	**0.100**	26.498
COST2	**0.779**	**0.144**	**0.191**	18.721	11.511	2.709	27.435	**0.100**	26.484
COST3	**0.777**	**0.142**	**0.189**	18.594	11.408	2.709	27.441	**0.100**	26.468

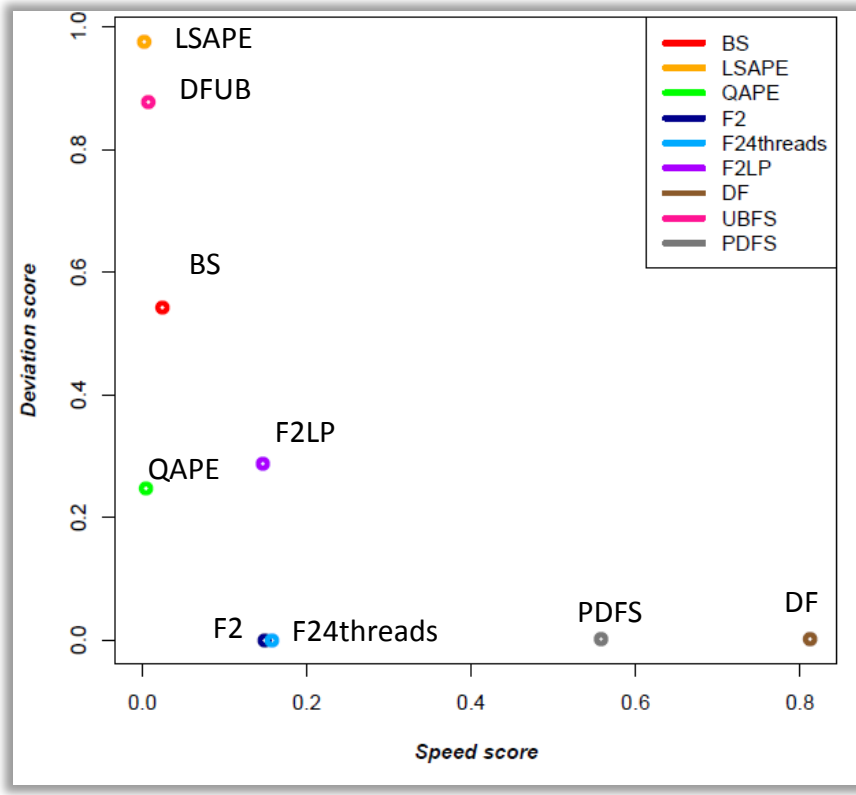
Acyclic - Deviation versus Running Time



Cost 1

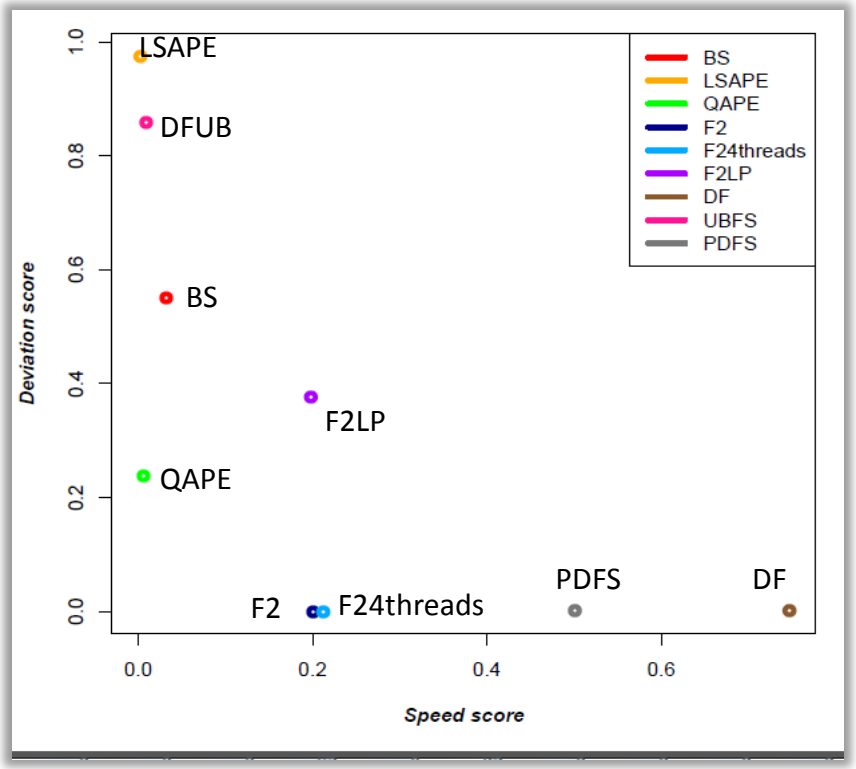


Cost 2

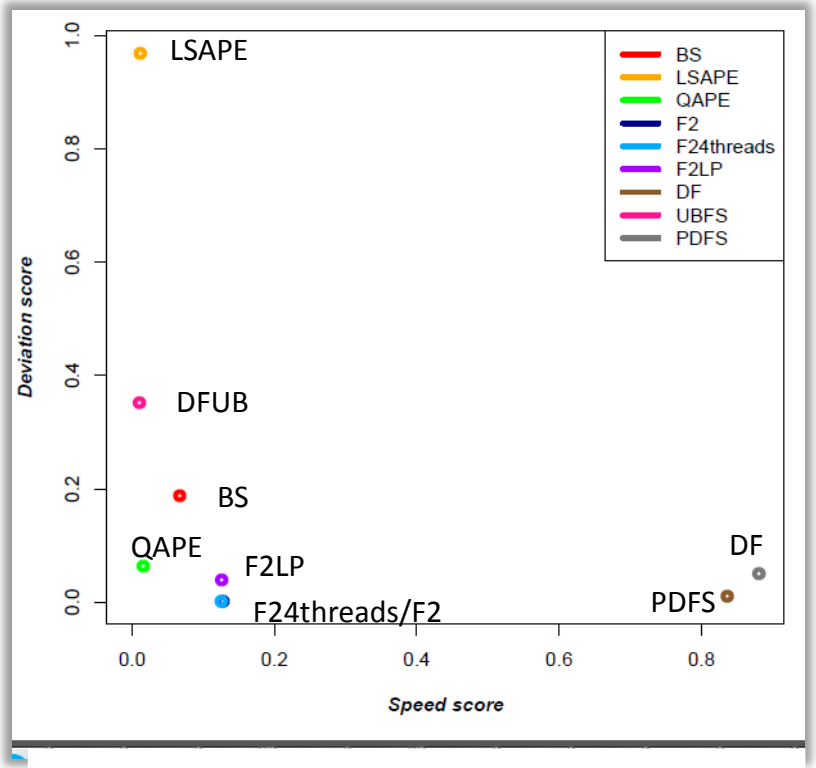


Cost 3

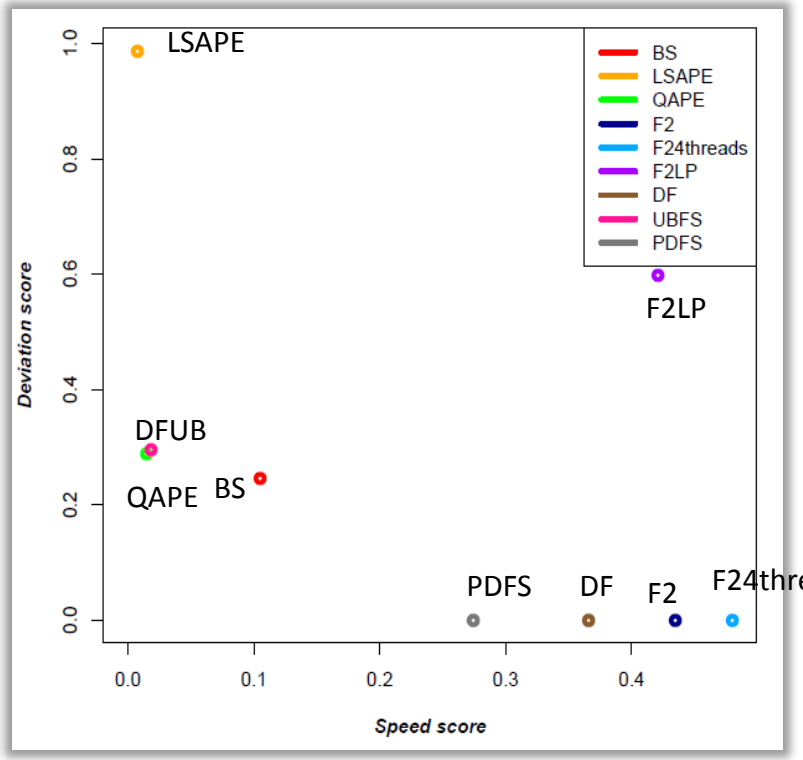
Alkane - Deviation versus Running Time



Cost 1

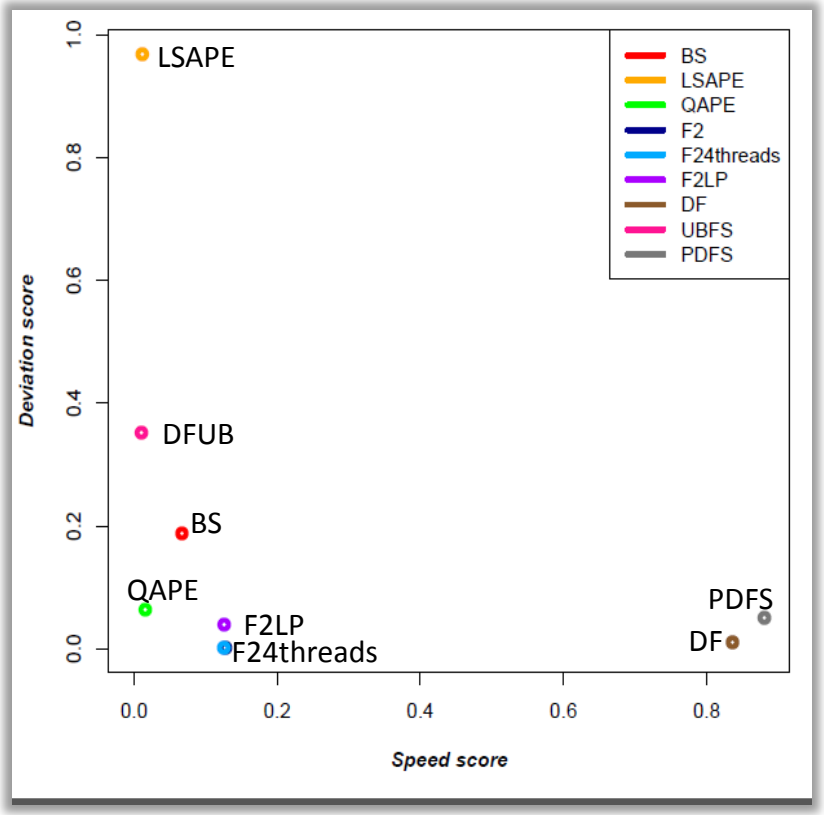


Cost 2

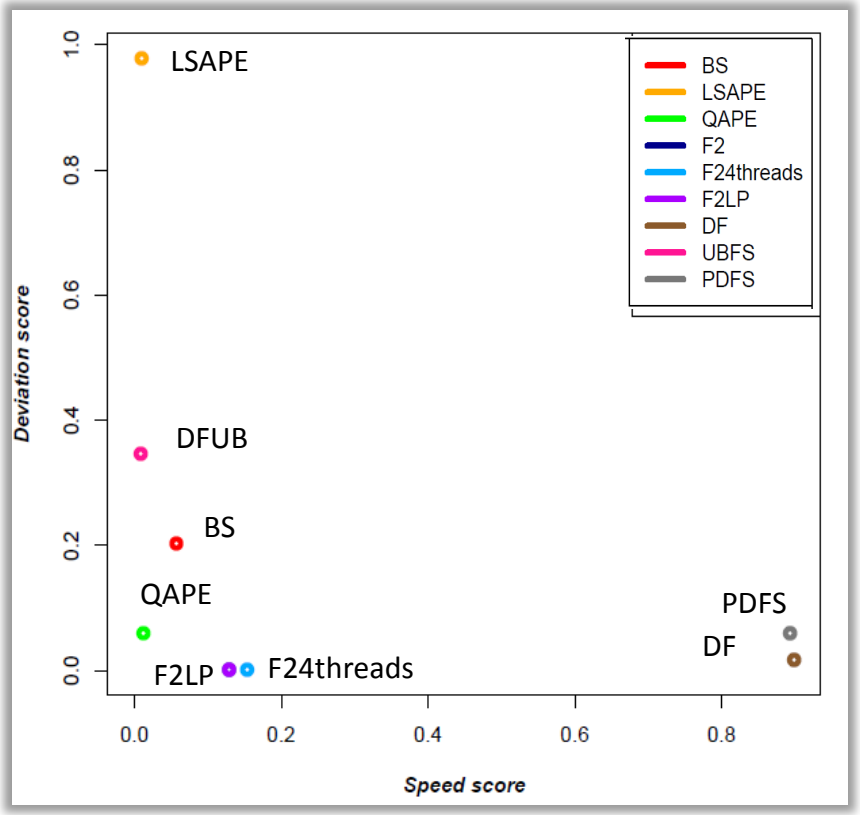


Cost 3

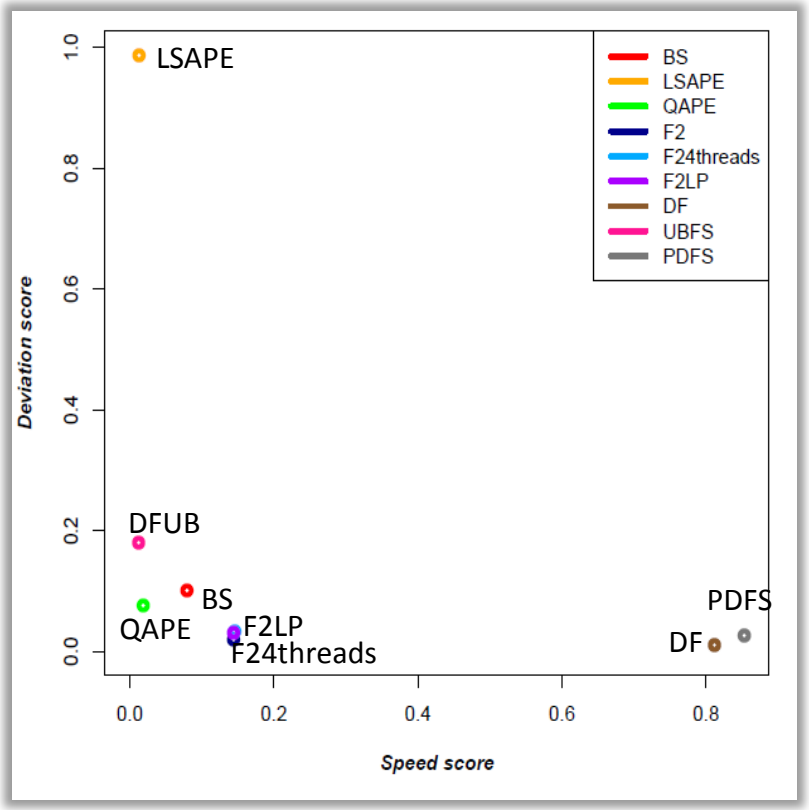
MAO - Deviation versus Running Time



Cost 1

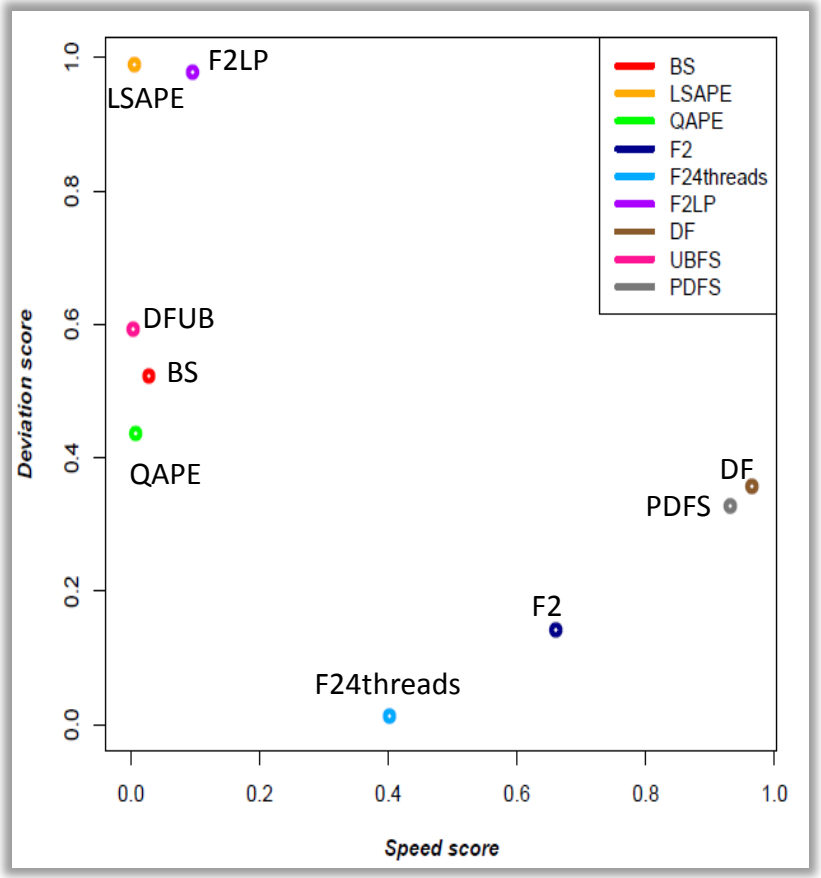


Cost 2

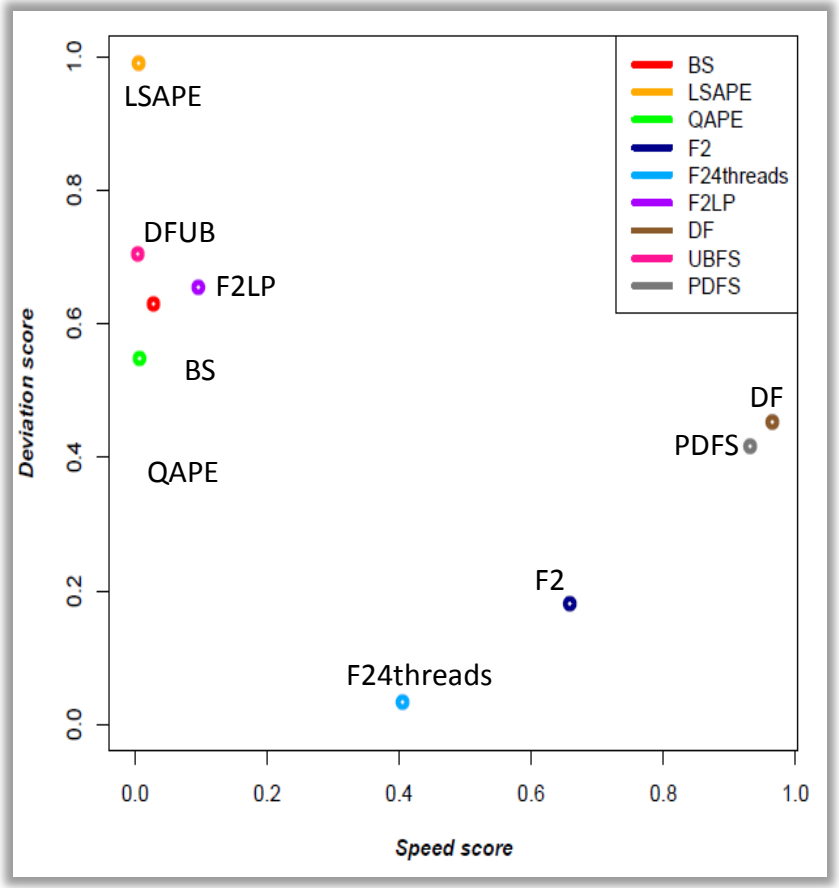


Cost 3

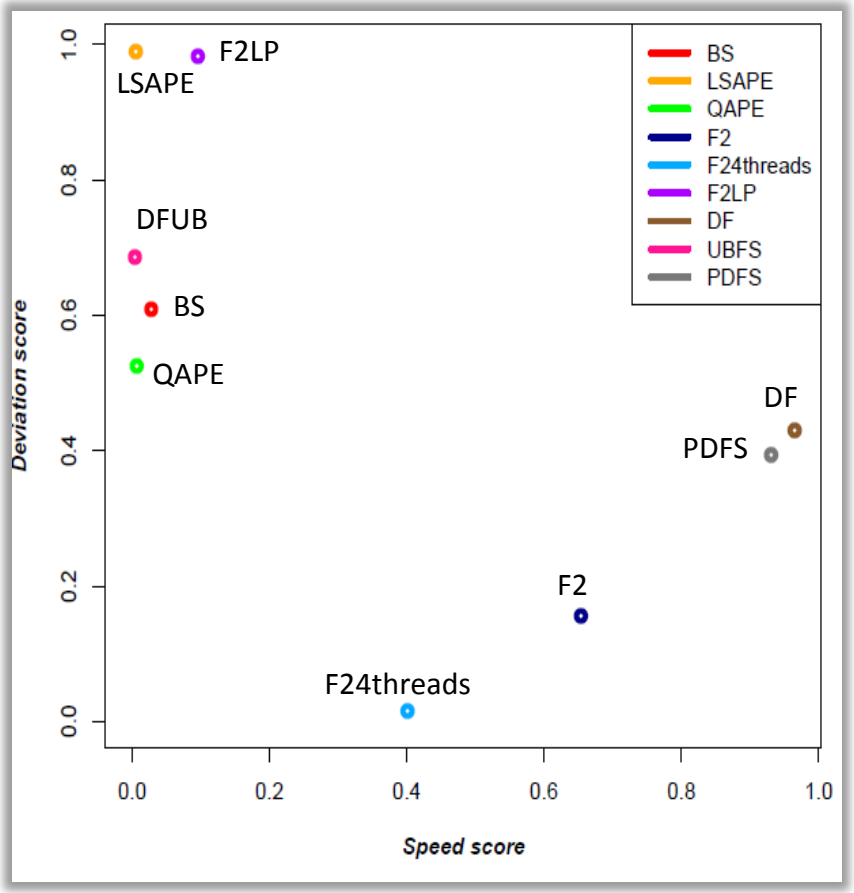
PAH - Deviation versus Running Time



Cost 1



Cost 2



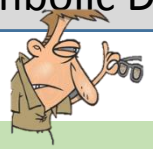
Cost 3

Conclusion 3

- Changing the costs does not have influence on the algorithms' behavior
- F24threads was the best on all datasets
- QAPE, DF and PDFS outperformed well on all datasets (except)

Outline

- Reminder
- Results
  - Symbolic Databases
    - Mutagenicity
    - Acyclic, Alkane and Mao
  - Numeric Databases
    - GREC
    - CMU
- Conclusion
- Perspectives



Facts

- LSAPE and QAPE approaches are based on heuristics only working on symbolic attributes:
  - They are excluded from this part of the contest

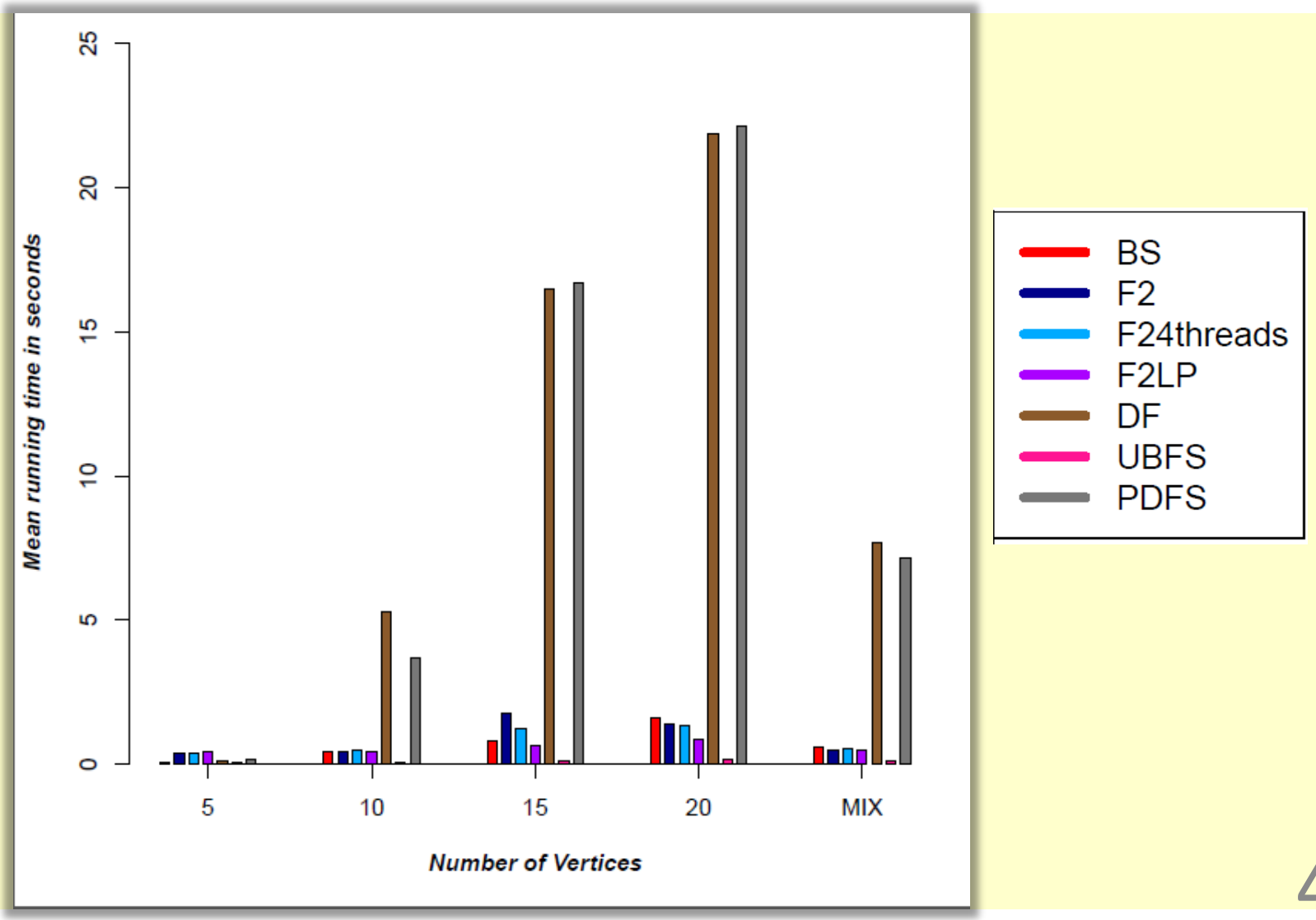
GREC - Deviation

		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
GREC-5	2.907	0	0	0	0	11.152	0
GREC-10	1.291	0	0	0.678	0	4.832	0
GREC-15	1.955	0	0	1.364	1.310	9.941	1.210
GREC-20	3.265	0	0	1.072	2.071	12.444	1.556
GREC-MIX	1.900	0	0	0.751	0.486	8.172	0.467

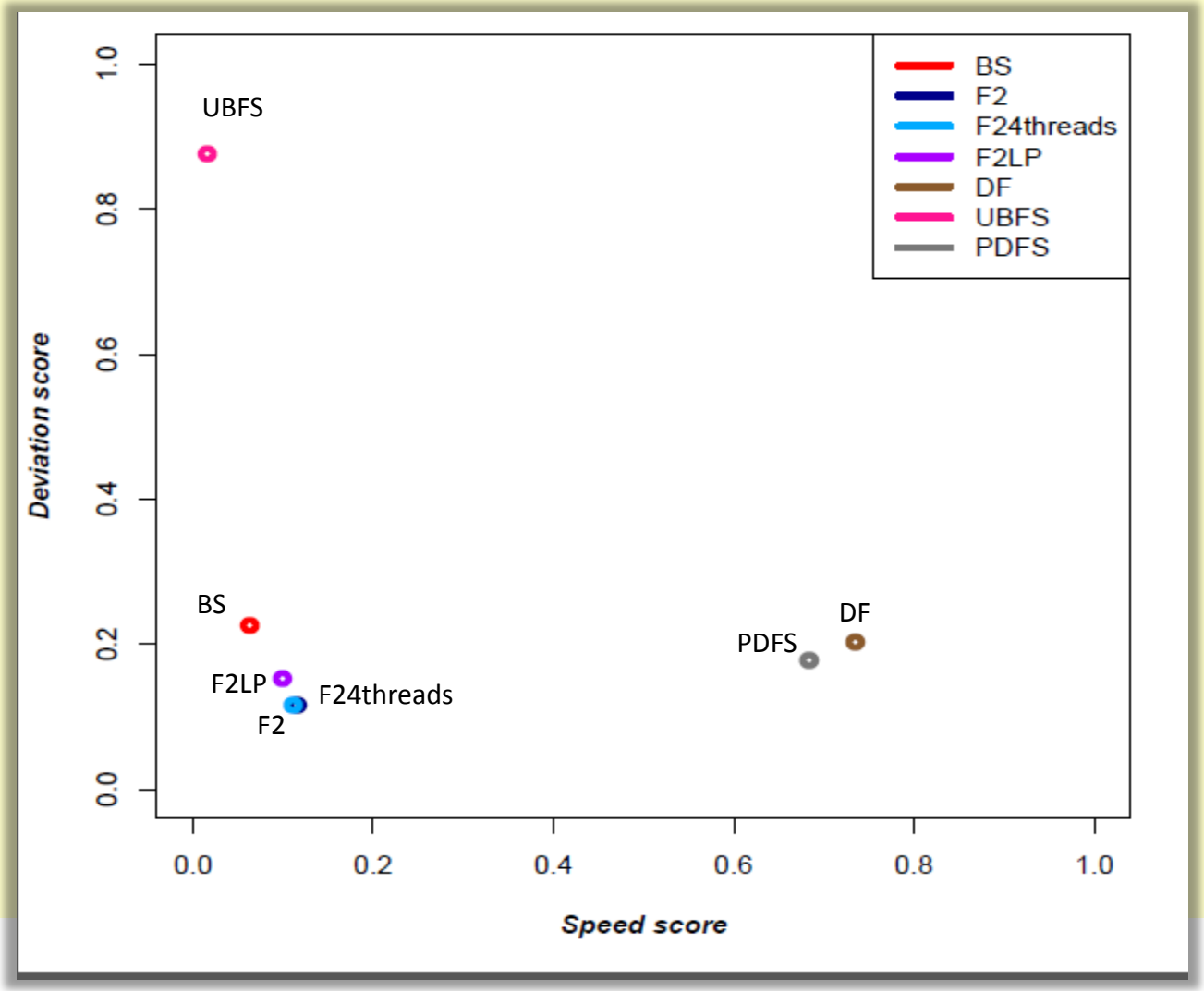
GREC - % Proved/Unproved Optimal Solutions

		Binary Linear Programming based Approaches			Branch-and-Bound based Approaches		
	BS	**F2**	**F24threads**	**F2LP**	**DF**	**DFUB**	**PDFS**
GREC-5	71	**100**	**100**	**100**	**100**	41	**100**
GREC-10	61	**100**	**100**	77	**100**	44	**100**
GREC-15	42	**100**	**100**	52	47	18	48
GREC-20	32	**100**	**100**	47	39	27	43
GREC-MIX	39	**100**	**100**	69	83	26	85

GREC - Running Time



To Sum Up: GREC - Deviation-Running Time



Conclusion 4

- F24threads was the best..
- It is easy to match graphs of GREC since the deviation of all the methods is quite low

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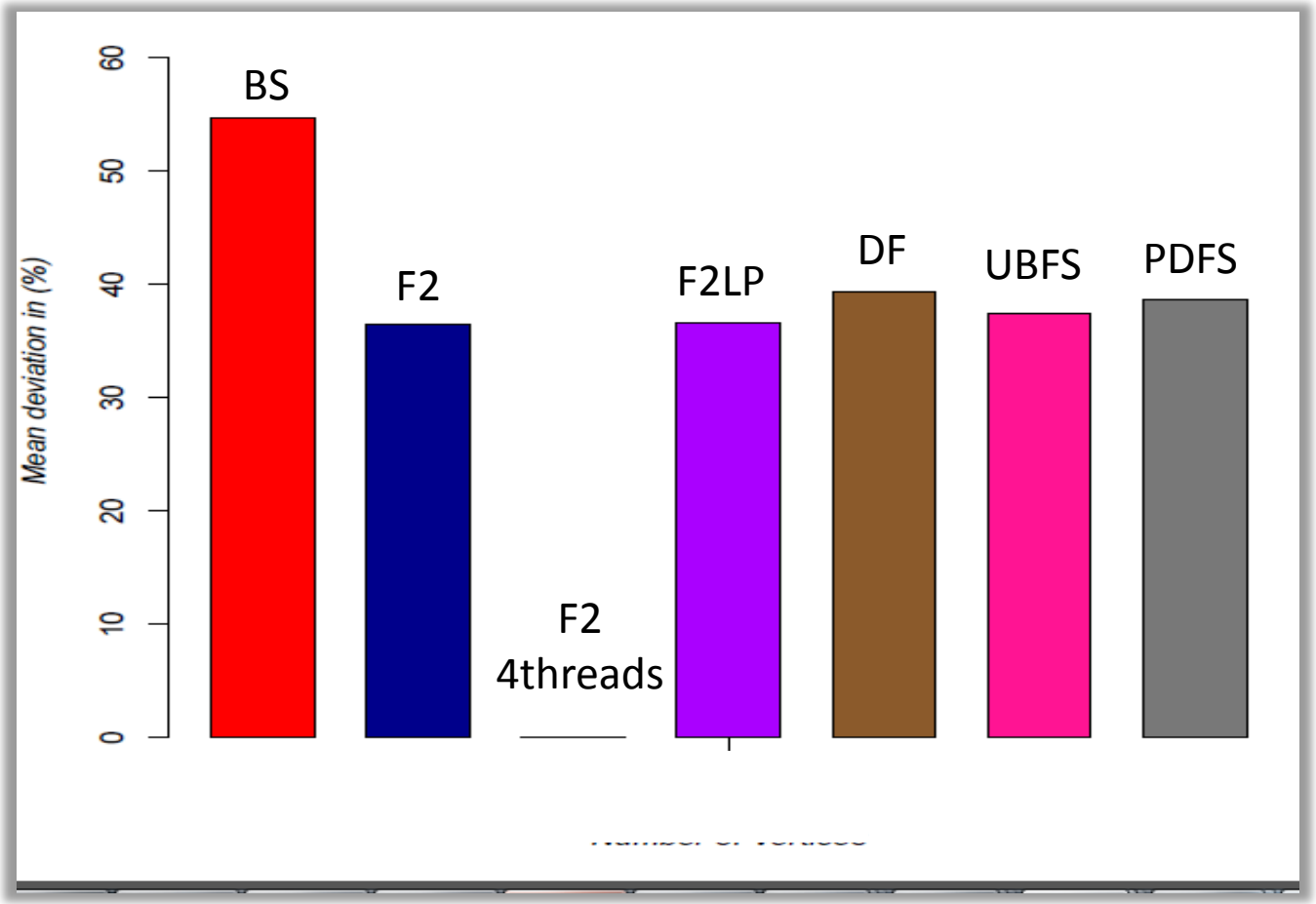
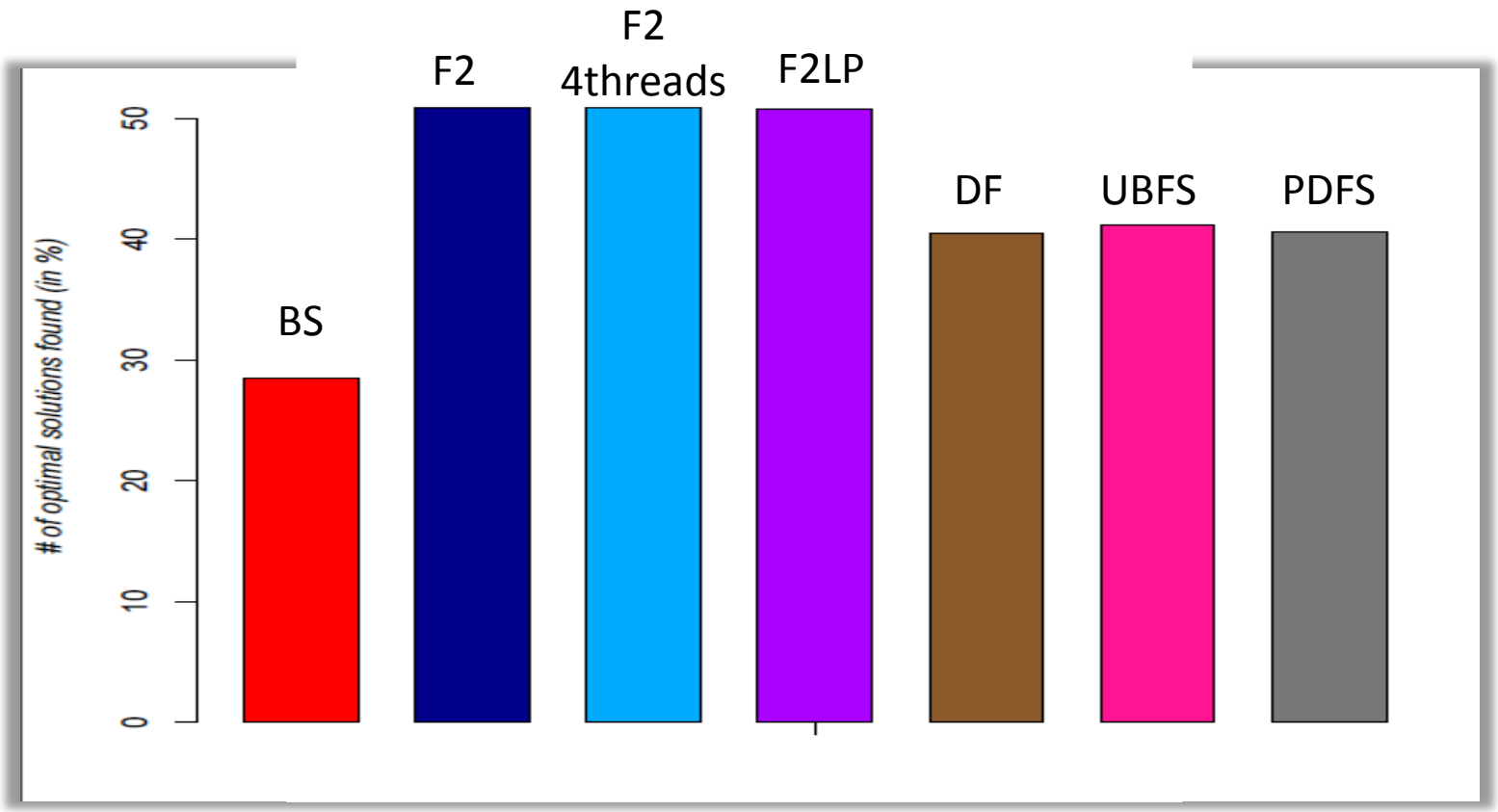
CMU - Deviation

BS	F2	F24threads	F2LP	DF	DFUB	PDFS
54.636	36.469	**0**	36.625	39.313	37.504	38.641



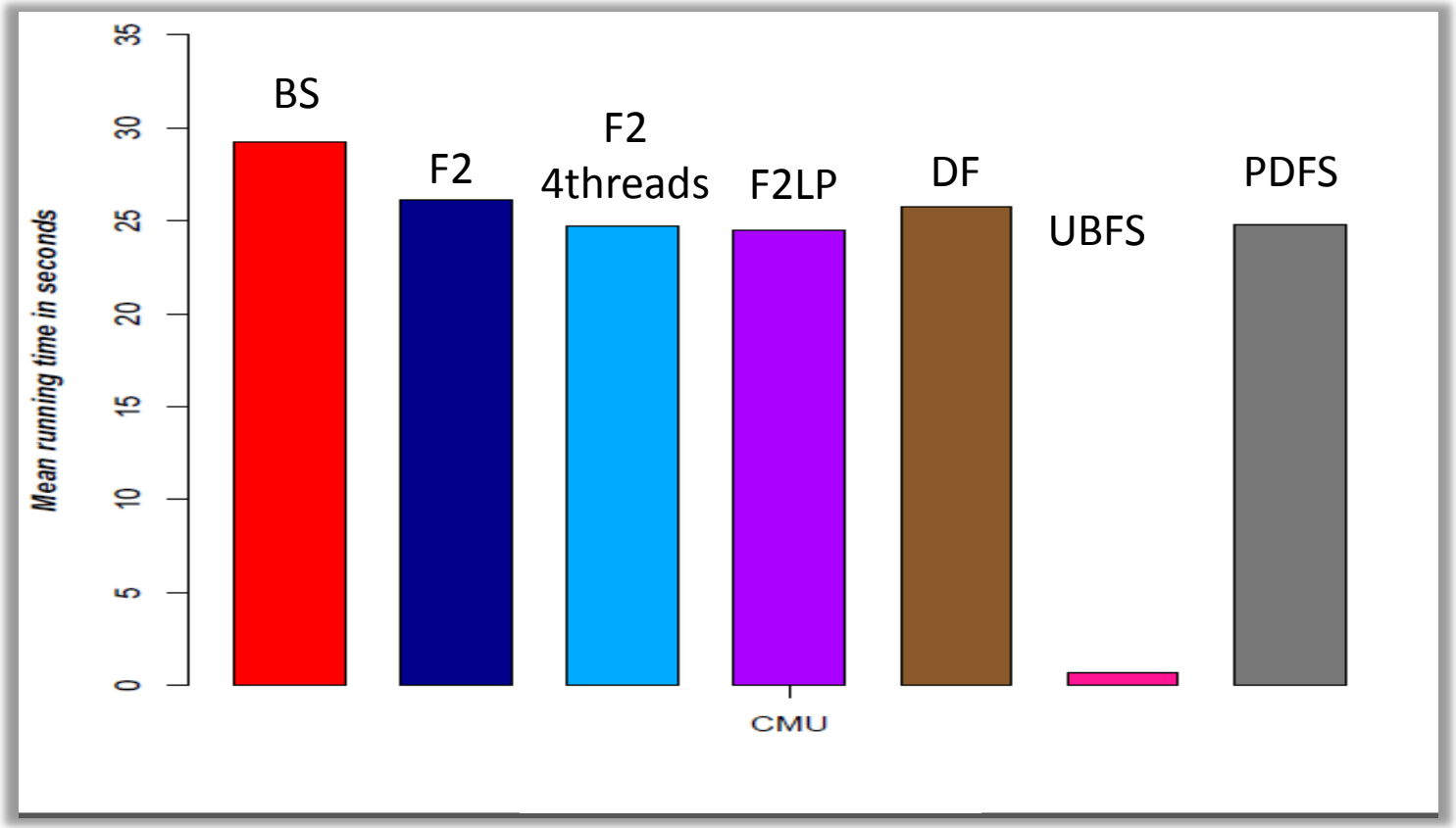
CMU - % Proved/Unproved Optimal Solutions

BS	F2	F24threads	F2LP	DF	DFUB	PDFS
28.484	50.909	**50.909**	50.757	40.454	41.212	40.606

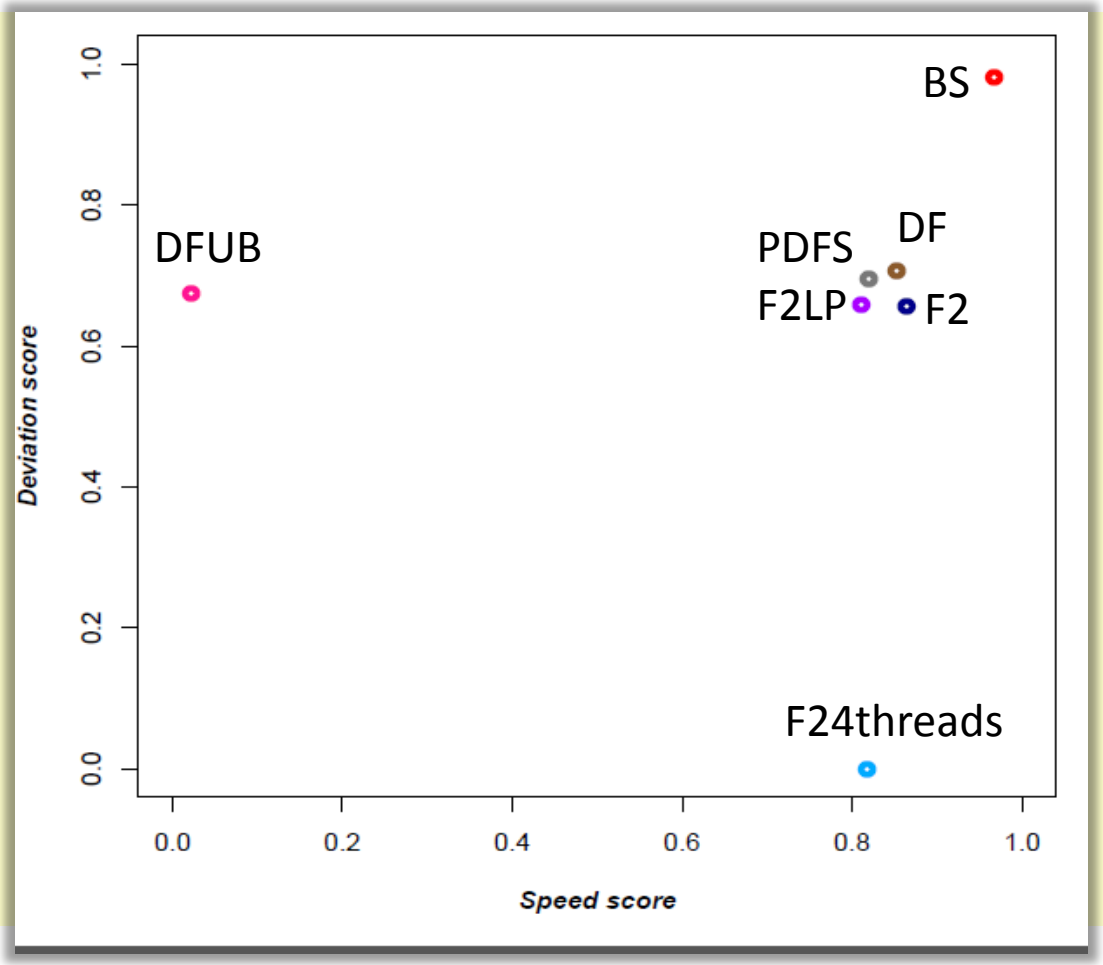


CMU - Running Time

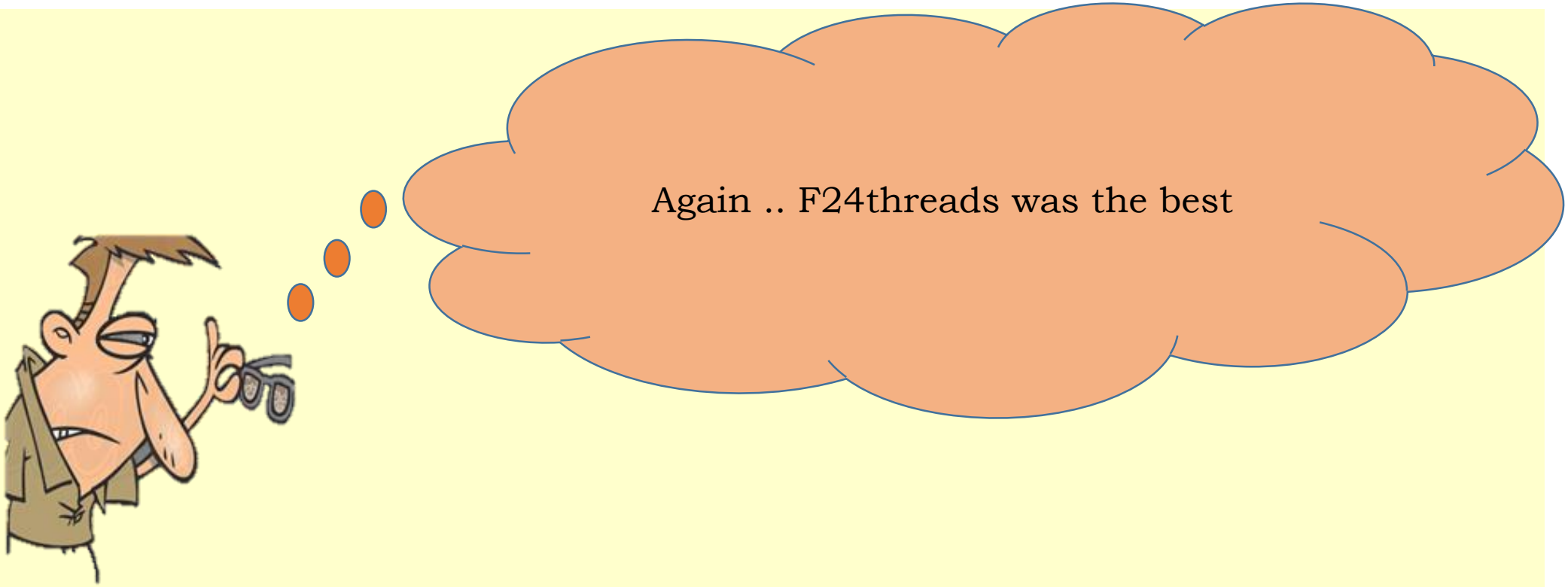
BS	F2	F24threads	F2LP	DF	DFUB	PDFS
29.235	26.128	**24.708**	24.516	25.773	0.657	24.788



To Sum Up: CMU - Deviation versus Running Time



Conclusion 4



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Conclusions

- **The winners:**
  - **F24threads** was the most precise algorithm
    - Limitations: it needs more time to output feasible solutions when increasing the size of graphs «MUTA-60 and MUTA-70»
  - **QAPE** was the most precise approximate algorithm
    - Since we don't have all the optimal solutions it's hard to tell how far are its solutions from the optimal ones
    - Still not adapted to work with numeric attributes
- **DF and PDFS** are highly dependant on the bipartite matching algorithm (used as a lower bound)
  - It will be improved

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Perspectives

- **More challenging datasets**
  - To have all the optimal solutions of the datasets.
  - Having bigger sizes of graphs
  - More dense graphs
  - Different types of attributes

- **Methods:**
  - There is still no method that can match more than 40 nodes with really good deviation → (compared to the optimal)

- Study the influence of costs on the methods

Thanks