New Benchmark Instances for the Steiner Problem in Graphs

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August 24, 2001

Abstract. We propose in this work 50 new test instances for the Steiner problem in graphs. These instances are characterized by large integrality gaps and symmetry aspects which make them harder to both exact methods and heuristics than the test problems currently in use for the evaluation and comparison of existing and newly developed algorithms. Our computational results indicate that these new instances are not amenable to reductions by current preprocessing techniques and that not only do the linear programming lower bounds show large gaps, but they are also hard to be computed. State-of-the-art heuristics, which found optimal solutions for almost all test instances currently in use, faced much more difficulties for the new instances. Fewer optimal solutions were found and the numerical results are more discriminant, allowing a better assessment of the effectiveness and the relative behavior of different heuristics.

Keywords: Steiner problem in graphs, benchmark instances, test instances, algorithms

1. Introduction

Let $G = (V, E)$ be a connected undirected graph, where V is the set of nodes and E denotes the set of edges. Given a non-negative weight function $w : E \rightarrow \mathbb{R}_+$ associated with its edges and a subset $X \subseteq V$ of terminal nodes, the Steiner problem in graphs (SPG) consists in finding a minimum weighted subtree of G spanning all nodes in X. The solution of SPG is a Steiner minimum tree. This is one of the most widely studied NP-hard problems, with many applications.

Three sets of benchmark instances are commonly used in the literature to assess the performance of algorithms for the SPG: instances available from the online repository OR-Library (Beasley, 1990), the "incidence" instances of Duin (1994) (see also (Duin and Voss, 1997)), and the VLSI instances of Koch and Martin (1998). All these instances are available from the SteinLib repository (Koch et al., 2001). However, these instances are rapidly becoming inadequate for benchmarking, for the following reasons:

– They have already been solved to optimality, with the exception of a few of the larger incidence instances (Duin, 1994; Koch and Martin, 1998;

Lucena and Beasley, 1998; Uchoa et al., 1999; Polzin and Vahdati, 2000; Poggi et al., 2001b). In fact, optimality can be proven within seconds in most cases. These instances are not challenging enough to stimulate further development of exact algorithms.

– Metaheuristics can easily find optimal solutions to a large portion of these instances (Duin and Voss, 1997; Duin and Voss, 1999; Gendreau et al., 1999; Martins et al., 2000; Ribeiro and Souza, 2000; Bastos and Ribeiro, 2001; Ribeiro et al., 2001). It is becoming increasingly hard to compare different metaheuristics properly. Deciding among different variants, parameter values, and implementation choices is also difficult, since they often lead to quite similar solutions, which are frequently optimal.

This paper proposes three new series of benchmark instances that will hopefully lead to a better assessment of exact and approximate algorithms for the SPG. Even though some of them are somewhat artificial, we believe they can play an important role in the development of algorithms whose ultimate goal is solving real-world instances. Algorithms that can cope with a variety of artificially hard instances tend to be very robust.

Our first goal was to design instances hard to be solved exactly. Current state-of-the-art exact algorithms are based on linear programming formulations that yield very tight bounds for most existing benchmark instances. They can solve several of these instances to optimality without branching. Even when branching is necessary, it is often possible to reduce the problem size significantly using reduction tests and fixation by reduced costs. Therefore, we tried to create instances with large duality gaps. To make them even harder, we introduced various degrees of symmetry, both in the structure of the underlying graphs and in terminal placement. In practice, symmetry increases the number of nodes in the search trees of branch-and-bound algorithms, since LP-based lower bounds tend to improve very slowly as branchings are performed.

The other design goal was to make the instances challenging also for metaheuristics. For each instance originally created, we generated another one with the same structure, but with perturbed edge weights. Since this results in instances with a much smaller number of optimal solutions, finding one of them by usual heuristic search methods tends to be a harder task.

Three classes of instances with a total of 50 reasonably small test problems are proposed and described in the next section. The number of nodes in each graph ranges from 64 to 4096, while the number of edges ranges from 128 to 28512. This means that, although much harder, our instances are not bigger than those currently in use. Section 3 presents some computational results and discusses the effectiveness of the new instances in terms of achieving their goal. Concluding remarks are made in Section 4.

2. Instances

2.1. HYPERCUBE (hc)

Graphs in this series are d-dimensional hypercubes, with $d \in \{6,\dots,12\}$. For each value of d, the corresponding graph has 2^d nodes and $d \cdot 2^{d-1}$ edges. These graphs are bipartite, and both partitions have the same number of nodes. The vertices in one of such subsets become terminals ($|X| = 2^{d-1}$). Edge weights in the originally created instances are unitary. The perturbed instances have integer edge weights randomly chosen from a uniform distribution in the interval $[100,110]$. These instances seem to be extremely difficult for existing algorithms. For example, using the branch-and-ascent algorithm proposed by Poggi et al. (2001b), we could not solve to optimality the instances with more than 128 nodes. Duality gaps are large and symmetry makes traditional branching schemes much less effective.

The naming convention is hc$d$[u|p], where u stands for "unperturbed" and p for "perturbed". For example, hc8u corresponds to an 8-dimensional hypercube with unperturbed weights. The pseudocode in Figure 1 describes the algorithm applied for the construction of these instances. We denote by $a \otimes b$ the integer number obtained by the exclusive-or operation between the binary representations of the integers a and b. To make the description of the algorithm simpler, the nodes of the d-dimensional hypercube are indexed by $i = 0,1,\dots,2^{d-1}-1$, instead of by $i = 1,2,\dots,2^{d-1}$. Then, $i \otimes 2^k$ gives the index of each neighbor of node i, for $k = 0,\dots,d-1$. Figure 2 shows what hc3u (a three-dimensional hypercubic instance) would look like.

```
E ← ∅
V ← ∅
X ← {0}
for i = 0,...,2^d − 1 do
    V ← V ∪ {i}
    for k = 0,...,d − 1 do
        j ← i ⊗ 2^k
        if i ∉ X then X ← X ∪ {j}
        w_{i,j} ← 1
        if (i, j) ∉ E then E ← E ∪ {(i, j)}
    end_for
end_for
```

Figure 1. Algorithm for the generation of the hypercube instances.

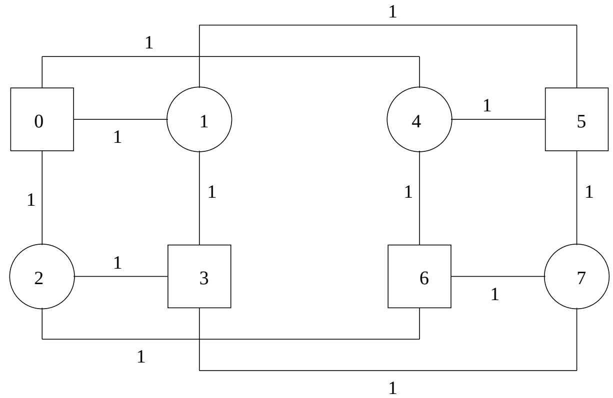

Figure 2. Graph associated with the hypercube instance hc3u.

2.2. CODE COVERING (cc)

Let V_q^n be the set of all n-dimensional vectors whose components are integers in the interval $[0, q-1]$. The *Code Covering Problem* (CCP) is defined as follows: given V_q^n and a positive integer r, find a minimum cardinality subset C of V_q^n such that there exists a vector $x \in C$ with $d(x,y) \leq r$ for all $y \in V_q^n$ (where d denotes the Hamming distance). This NP-hard problem (Lint, 1975) is equivalent to finding a minimum dominating set in a graph $G = (V_q^n, E)$, where $(x,y) \in E$ whenever $d(x,y) \leq r$.

We created instances for the SPG using 13 of such graphs and taking as the set of terminals a solution (i.e., a dominating set) obtained by the tabu search algorithm of Poggi and Souza (1999). Edges have incidence weights so as to make preprocessing ineffective, following Duin (1994) and Duin and Voss (1997). In the unperturbed case, this means that an edge has weight equal to 1 if it connects non-terminals, 2 if it is incident to a single terminal, and 3 if it connects two terminals. The perturbed case follows the same principle, but with integral weights uniformly distributed in the intervals $[100, 110]$, $[200, 210]$, or $[300, 310]$, depending on the number of terminals incident to an edge.

Although these instances do challenge current exact algorithms, they are not as hard as the hc instances. The graphs in this case are still very symmetric, but terminal placement is not.

The naming convention is cc$n$-q[u|p] (the value of r is omitted because we have used only $r = 1$). For example, cc3-4u corresponds to an unperturbed instance derived from a CCP with $n = 3$ and $q = 4$ (and $r = 1$). Figure 3 shows what the code covering instance cc3-2u with $q = 2$ and $n = 3$ would look like.

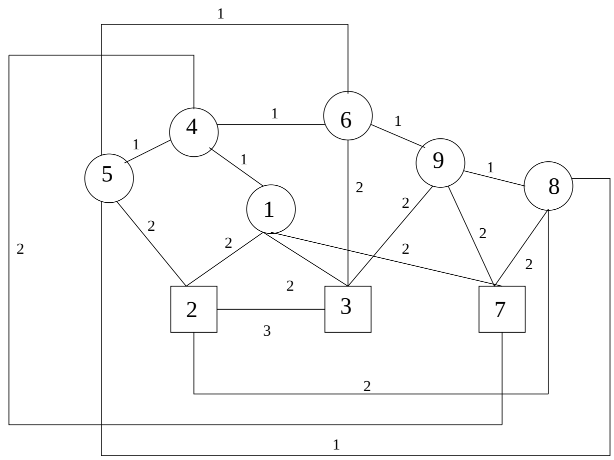

Figure 3. Code covering instance cc3-2u.

2.3. BIPARTITE (bip)

This series contains ten instances defined on irregular bipartite graphs, with one of the bipartition-defining vertex subsets acting as the set of terminals. These graphs are derived from random instances of the set covering problem (SCP) from the OR-Library (Beasley, 1990). Given an instance I of SCP with m rows and n columns, we build an instance I' for the SPG as follows. There is a terminal in I' associated with each row i in I. Similarly, each non-terminal node in I' is associated with a column j in I. Whenever row i covers column j, there is an edge linking terminal i to the non-terminal node j in I'. The resulting graph has $m+n$ vertices, m terminals, and as many edges as nonzero entries in the coefficient matrix of the SCP instance I. Edge weights are unitary in the unperturbed case and uniformly distributed in the interval $[100,110]$ for the instances with perturbations.

The naming convention is bip$I$[u|p], where I is the name of the SCP instance (minus the scp prefix). For example, bipe2u is the SPG instance with unperturbed weights associated with instance scpe2 of the OR-Library. Figure 4 shows what a bipartite instance with $m=3$ and $n=4$ would look like.

Our motivation in creating this series was to have instances with a certain structure (bipartite), but without the artificial symmetry found in the previous two classes. Using SCP instances is no better or worse than generating random bipartite graphs from scratch, but the OR-Library instances have the advantage of being already publicly available.

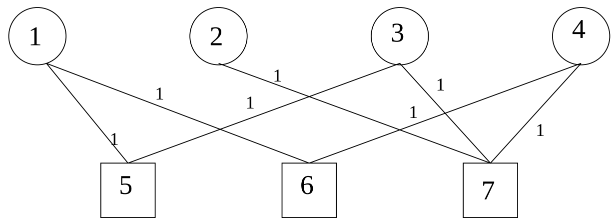

Figure 4. An example of bipartite instance.

3. Experimental results

This section presents some preliminary results on the new instances proposed. We have conducted some experiments to determine if they are indeed hard to be solved.

One of the most important practical techniques for the solution of SPG instances is the preprocessing phase, which consists of applying tests that try to eliminate some edges or vertices from the instance before any optimization algorithm is invoked. The hypercube and code covering instances could not be reduced, either by the traditional reduction tests of Duin and Volgenant (1989) or by the recent tests proposed by Uchoa et al. (1999). The sparse bipartite instances can be slightly reduced by some very simple tests. For instance, in the case of instance depicted in Figure 4, vertex 2 and its incident edge can be removed by the NTD1 Non-Terminal Degree 1 test. In the same figure, vertex 3 could be removed and its incident edges replaced by a single edge with cost equal to 2 from vertex 5 to 7 by the NTD2 test. Table I shows the dimensions of the bipartite instances before and after preprocessing. Although all tests were applied, only the TD1, NTD1, and NTD2 tests described by Duin and Volgenant (1989) lead to some reductions.

Table I. Dimensions of the bipartite instances before and after preprocessing.

Instance	before preprocessing			after preprocessing		
	$\|V\|$	$\|E\|$	$\|X\|$	$\|V\|$	$\|E\|$	$\|X\|$
bipe2u	550	5013	50	550	5013	50
bip42u	1200	3982	200	990	3610	200
bip62u	1200	10002	200	1199	10000	200
bip52u	2200	7997	200	1819	7326	200
bipa2u	3300	18073	300	3140	17795	300
bipe2p	550	5013	50	550	5013	50
bip42p	1200	3982	200	990	3619	200
bip62p	1200	10002	200	1199	10000	200
bip52p	2200	7997	200	1819	7336	200
bipa2p	3300	18073	300	3140	17797	300

Tables II to IV present the results obtained for each of the new classes of instances. For each instance, we first report its dimensions. Next, we give the weights of the solutions found by five different heuristics: (SPH) shortest-path heuristic (Takahashi and Matsuyama, 1980), (HGP) hybrid GRASP with perturbations (Ribeiro et al., 2001), (HGP-PR) hybrid GRASP with perturbations and adaptive path-relinking (Ribeiro et al., 2001), (RTS) reactive tabu search (Bastos and Ribeiro, 2001), and (RTS-PR) reactive tabu search with path-relinking (Bastos and Ribeiro, 2001). These implementations were selected only because they were readily available to us. The shortest-path heuristic is included in this study only to indicate to the reader how a simple and fast approximate algorithm performs for these instances. Results for the bipartite instances in Table IV were obtained after preprocessing.

We now comment on the relative effectiveness of these heuristics when applied to the new classes of instances. We stress that our goal here is not to try to establish the superiority of one heuristic over the others. Instead, we want to show that the new instances provide a test bed on which insightful conclusions can be easily drawn, which is not always the case for the instances currently available in the literature.

Results in italics emphasize the best solution value among those obtained by the five heuristics. HGP-PR is clearly the heuristic with the best performance, finding the best solution for all but three instances. Comparing the implementations of metaheuristics which do not make use of path-relinking, HGP is never less effective than RTS for the unperturbed instances, which indicates that it is more suited to instances with many global optima. On the other hand, RTS performs better than HGP for most perturbed instances.

We also give in these tables the linear programming lower bound (LP) obtained by solving the linear relaxation of the directed cut formulation (Wong, 1984), the best upper bound we could find, and an estimate of the duality gap given by the percentual difference between these values (gap). The upper bound was obtained with the GHLS3 variant (Poggi et al., 2001a) of the hybrid GRASP with perturbations and adaptive path-relinking (HGP-PR). It uses a more powerful local search based on key-nodes and a larger pool of elite solutions. Results in bold face indicate optimal values proved by the algorithm described by Poggi et al. (2001b).

4. Concluding remarks

The results in Tables I to IV clearly indicate that the new instances proposed in this work are not amenable to reductions by current preprocessing techniques and that the linear programming upper bounds have large gaps and are hard to be computed. State-of-the-art heuristics, which found optimal solutions for almost all instances currently in use, faced much more difficulties

Table II. Hypercube instances

Instance	$\lvert V \rvert$	$\lvert E \rvert$	$\lvert X \rvert$	SPH	HGP	HGP-PR	RTS	RTS-PR	LP	GHLS3	gap (%)
hc6u	64	192	32	41	*39*	*39*	*39*	*39*	37.1	**39**	4.87
hc7u	128	448	64	80	*77*	*77*	*77*	*77*	73.4	**77**	4.68
hc8u	256	1024	128	157	*149*	*149*	151	151	145.1	148	≤ 1.96
hc9u	512	2304	256	319	*296*	*296*	304	304	286.8	292	≤ 1.78
hc10u	1024	5120	512	627	*588*	*588*	606	606	567.7	582	≤ 2.46
hc11u	2048	11264	1024	1219	*1173*	*1173*	1200	1200	≥1125.2	1162	≤ 3.17
hc12u	4096	24576	2048	2427	*2336*	*2336*	2396	2396	≥2201.1	2303	≤ 4.42
hc6p	64	192	32	4302	4017	*4003*	*4003*	*4003*	3867.6	**4003**	3.38
hc7p	128	448	64	8384	7932	*7905*	7909	7909	7646.8	**7905**	3.27
hc8p	256	1024	128	16746	15637	*15376*	15573	15526	15115.7	15322	≤ 1.35
hc9p	512	2304	256	32509	31108	*30572*	30996	30920	29877.6	30258	≤ 1.26
hc10p	1024	5120	512	64472	61905	*61030*	61633	61605	59213.4	60494	≤ 2.12
hc11p	2048	11264	1024	128204	123129	*120804*	122741	122741	117388.7	120096	≤ 2.25
hc12p	4096	24576	2048	253825	244674	*243390*	244477	244477	≥232709.0	238673	≤ 2.50

The time limit for the computation of the LP bound was set at 6 hours on a 400 MHz Pentium II machine.

Table III. Code cover instances

Instance	$\lvert V \rvert$	$\lvert E \rvert$	$\lvert X \rvert$	SPH	HGP	HGP-PR	RTS	RTS-PR	LP	GHLS3	gap (%)
cc6-2u	64	192	12	*32*	*32*	*32*	*32*	*32*	29.8	**32**	6.88
cc3-4u	64	288	8	*23*	*23*	*23*	*23*	*23*	21.0	**23**	8.70
cc3-5u	125	750	13	*36*	*36*	*36*	*36*	*36*	≥32.8	**36**	≤ 8.89
cc5-3u	243	1215	27	76	72	*71*	74	73	69.5	**71**	2.11
cc9-2u	512	2304	64	187	*171*	*171*	178	*171*	≥162.7	167	≤ 2.57
cc6-3u	729	4368	76	217	201	*198*	209	206	≥194.1	197	≤ 1.47
cc3-10u	1000	13500	50	132	*126*	*126*	130	129	123.8	**125**	0.96
cc10-2u	1024	5120	135	381	349	*346*	362	359	≥332.4	342	≤ 2.81
cc3-11u	1331	19965	61	163	*154*	*154*	158	157	≥151.0	153	≤ 1.31
cc3-12u	1728	28512	74	191	*186*	*186*	187	187	≥182.0	186	≤ 2.15
cc11-2u	2048	11263	244	687	624	*619*	669	651	≥600.5	614	≤ 2.20
cc7-3u	2187	15308	222	612	562	*554*	598	588	≥534.1	552	≤ 3.24
cc12-2u	4096	24574	473	1315	1201	*1184*	1287	1255	≥1141.0	1179	≤ 3.22
cc6-2p	64	192	12	3388	*3271*	*3271*	*3271*	*3271*	3078.3	**3271**	5.89
cc3-4p	64	288	8	2349	*2338*	*2338*	*2338*	*2338*	2194.0	**2338**	6.16
cc3-5p	125	750	13	3673	3667	*3661*	3664	3664	≥3384.6	**3661**	≤ 7.55
cc5-3p	243	1215	27	8266	7491	*7404*	7484	7484	≥7117.8	7299	≤ 2.48
cc9-2p	512	2304	64	18704	17836	*17376*	17946	17904	≥16766.0	17296	≤ 3.06
cc6-3p	729	4368	76	22680	20850	*20554*	21060	20657	≥20064.1	20458	≤ 1.93
cc3-10p	1000	13500	50	14149	13084	13061	13118	*13003*	≥12663.6	12860	≤ 1.53
cc10-2p	1024	5120	135	38608	36552	*35867*	37234	36545	≥34297.2	35466	≤ 3.30
cc3-11p	1331	19965	61	17111	15924	*15728*	15940	15917	≥15436.8	15609	≤ 1.10
cc3-12p	1728	28512	74	20626	19285	19167	19201	*19159*	≥18634.9	18838	≤ 1.08
cc11-2p	2048	11263	244	70666	66073	*64334*	68486	67328	≥61905.0	63841	≤ 3.03
cc7-3p	2187	15308	222	63339	59005	*57601*	61190	60303	≥55071.9	57339	≤ 3.95
cc12-2p	4096	24574	473	135953	126541	*122928*	131778	128015	≥117884.5	121772	≤ 3.19

The time limit for the computation of the LP bound was set at 6 hours on a 400 MHz Pentium II machine.

for the new instances. Fewer optimal solutions were found and the numerical results are more discriminant, allowing a better assessment of the effectiveness and the relative behavior of different heuristics. The new instances have been available at the SteinLib repository (Koch et al., 2001) since July 2001.

Table IV. Bipartite instances

Instance	$\|V\|$	$\|E\|$	$\|X\|$	SPH	HGP	HGP-PR	RTS	RTS-PR	LP	GHLS3	gap (%)
bipe2u	550	5013	50	60	*55*	*55*	*55*	*55*	52.4	54	$\leq$ 2.96
bip42u	1200	3982	200	270	248	*239*	259	258	232.0	237	$\leq$ 2.11
bip62u	1200	10002	200	247	229	*227*	233	231	213.3	221	$\leq$ 3.48
bip52u	2200	7997	200	275	248	*247*	261	261	229.1	235	$\leq$ 2.51
bipa2u	3300	18073	300	385	358	*356*	371	367	$\geq$329.3	342	$\leq$ 3.71
bipe2p	550	5013	50	6334	5721	5684	5687	*5666*	5515.4	5660	$\leq$ 2.55
bip42p	1200	3982	200	28758	25737	*25175*	25833	25285	24373.8	24818	$\leq$ 1.79
bip62p	1200	10002	200	25267	23877	*23291*	23779	23500	22445.2	22944	$\leq$ 2.17
bip52p	2200	7997	200	29616	26137	*25415*	26079	25884	24186.3	24936	$\leq$ 3.01
bipa2p	3300	18073	300	40457	37368	*36439*	37415	37345	34685.7	35774	$\leq$ 3.04

The time limit for the computation of the LP bound was set at 6 hours on a 400 MHz Pentium II machine.

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