ug[SCIP-Jack, MPI]: A Massively Parallel Steiner Tree Solver

Daniel Rehfeldt · Yuji Shinano · Thorsten Koch Zuse Institute Berlin Technische Universität Berlin



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The Steiner Tree Problem in Graphs

Given:

- \triangleright G = (V, E): undirected graph
- \triangleright $T \subseteq V$: subset of vertices
- $\triangleright \ c \in \mathbb{R}_{>0}^{E}$: positive edge costs



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Steiner Tree Problem in Graphs (SPG)

Find a Steiner tree S in (G, T, c) with minimum edge costs $\sum_{e \in E(S)} c(e)$

SPG is one of the fundamental combinatorial optimization problems; decision variant is one of Karp's 21 \mathcal{NP} -complete problems.

Why not using a general MIP solver?

Consider (small-scale) network design instance with:

$$|V| = 12715$$

 $|E| = 41264$
 $|T| = 475$

- CPLEX 12.7.1: No optimal solution within 72 hours
- SCIP-Jack: Solves to optimality in 7.5 seconds

For larger problems CPLEX runs out of memory almost immediately (largest real-world instance SCIP-Jack solved so far has 64 million edges, 11 million vertices)



Network telecommunication design for Austrian cities, see *New Real-world Instances for the Steiner Tree Problem in Graphs* (Leitner et al., 2014)



Some real-world applications of Steiner trees:

- design of fiber optic networks
- prediction of tumor evolution
- deployment of drones
- computer vision
- wire routing
- computational biology
- ▷ ...



Rooted prize-collecting Steiner tree problem

E.g. An algorithmic framework for the exact solution of the prize-collecting Steiner tree problem (Ljubic et al., 2006)

Applications

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- design of fiber optic networks
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- ▷..



Rectilinear Steiner minimum tree problem

E.g. Phylogenetic analysis of multiprobe fluorescence in situ hybridization data from tumor cell populations (Chowdhury et al., 2013)

Applications

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Hop-constrained directed Steiner tree problem

E.g. Local Search for Hop-constrained Directed Steiner Tree Problem with Application to UAV-based Multi-target Surveillance (Burdakov, 2014)



Some real-world applications of Steiner trees:

- \triangleright design of fiber optic networks
- $\,\triangleright\,$ prediction of tumor evolution
- \triangleright deployment of drones
- ▷ computer vision
- \triangleright wire routing

 \triangleright . . .

computational biology



Maximum-weight connected subgraph problem

E.g. Efficient activity detection with max-subgraph search (Chen, Grauman, 2012)

Applications

Some real-world applications of Steiner trees:

- \triangleright design of fiber optic networks
- prediction of tumor evolution
- b deployment of drones
- computer vision
- write routing
- computational biology
- ▷ ...



Group Steiner tree problem

E.g. Rectilinear group Steiner trees and applications in VLSI design (Zachariasen, Rohe, 2003)



Some real-world applications of Steiner trees:

- design of fiber optic networks
- prediction of tumor evolution
- deployment of drones
- computer vision
- ▷ wire routing
- computational biology
- ▷ ...



Maximum-weight connected subgraph problem

E.g. Solving Generalized Maximum-Weight Connected Subgraph Problems for Network Enrichment Analysis (Loboda et al., 2016)



Some real-world applications of Steiner trees:

- ▷ design of fiber optic networks
- ▷ prediction of tumor evolution
- deployment of drones
- computer vision
- ▷ wire routing

▷ ...

computational biology



Maximum-weight connected subgraph problem

Real-world applications usually require variations of SPG

What we wanted: Solver for Steiner tree and many related problems

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... cutting plane algorithm based on flow balance directed-cut formulation:

Formulation

$$\begin{array}{ll} \min c^{T}y \\ y(\delta^{+}(W)) & \geqslant & 1 \\ y(\delta^{-}(v)) & \leqslant & y(\delta^{+}(v)) \\ y(\delta^{-}(v)) & \leqslant & y(\delta^{+}(v)) \\ y(\delta^{-}(v)) & \geqslant & y(a) \\ y(a) & \in & \{0,1\} \\ \end{array} \begin{array}{ll} \text{for all } w \in V \setminus T \\ for \ all \ a \in \delta^{+}(v), v \in V \setminus T \\ y(a) & \in & \{0,1\} \\ \end{array}$$

Framework



Some Facts about SCIP

\triangleright general setup

- plugin based system
- default plugins handle MIPs and nonconvex MINLPs
- support for branch-and-price and custom relaxations
- $\triangleright~$ documentation and guidelines
 - ▶ more than 500 000 lines of C code, 20% documentation
 - ► 36 000 assertions, 5 000 debug messages
 - HowTos: plugins types, debugging, automatic testing
 - 11 examples and 5 applications illustrating the use of SCIP
 - active mailing list scip@zib.de (300 members)
- ▷ interface and usability
 - user-friendly interactive shell
 - interfaces to AMPL, GAMS, ZIMPL, MATLAB, Python and Java
 - C++ wrapper classes
 - LP solvers: CLP, CPLEX, Gurobi, MOSEK, QSopt, SoPlex, Xpress
 - over 1600 parameters and 15 emphasis settings

(Some) Universities and Institutes using SCIP



about 8000 downloads per year

SCIP plus Jack



Development of SCIP-Jack has been joint work with: Gerald Gamrath · Thorsten Koch · Stephen J. Maher · Yuji Shinano

A Steiner class solver

SCIP-Jack can solve SPG and 12 related problems:

Abbreviation	Problem Name
SPG	Steiner tree problem in graphs
SAP	Steiner arborescence problem
RSMT	Rectilinear Steiner minimum tree problem
OARSMT	Obstacle-avoiding rectilinear Steiner minimum tree problem
NWSTP	Node-weighted Steiner tree problem
NWPTSTP	Node-weighted partial terminal Steiner tree problem
PCSTP	Prize-collecting Steiner tree problem
RPCSTP	Rooted prize-collecting Steiner tree problem
MWCSP	Maximum-weight connected subgraph problem
RMWCSP	Rooted maximum-weight connected subgraph problem
DCSTP	Degree-constrained Steiner tree problem
GSTP	Group Steiner tree problem
HCDSTP	Hop-constrained directed Steiner tree problem



SCIP-Jack works by combining generic and problem specific algorithms:



SCIP-Jack works by combining generic and problem specific algorithms:

- ▷ generic
 - extremely fast separator routine based on new max-flow implementation
 - all general methods provided by SCIP e.g., generic cutting planes
- problem specific
 - efficient transformations to Steiner arborescence problem (needed for applying generic separator)
 - preprocessing and propagation routines
 - primal and dual heuristics

SCIP-Jack



Performance of SCIP-Jack for SPG

SCIP-Jack is

- usually between two and three orders of magnitude faster than Jack-III (both using CPLEX 12.7.1 as LP-solver)
- ▷ fastest publicly available solver for SPG
- ▷ also fastest solver for several related problems...



The Parameterized Algorithms and Computational Experiments Challenge fixed-parameter tractable instances; more than 100 participants Setting: 3 tracks, 100 instances in each track, time limit 30 min.

- ▷ Track A: exact, few terminals; results on public instances:
 - ▶ Winner: 94/100 Iwata, Shigemura (NII, Japan)
 - ► SCIP-Jack/SoPlex: 93/100 3rd place
 - SCIP-Jack/CPLEX: 100/100
- ▷ Track B: exact, low treewidth; results on public instances:
 - ► SCIP-Jack/SoPlex: 98/100 1st place
 - SCIP-Jack/CPLEX: 99/100
 - best other: 84/100
- ▷ Track C: heuristic, mean ratio to best known upper bound:
 - ▶ Winner: 99.92 Ruiz, Cuevas, López, González (CIMAT, Mexico)
 - ► SCIP-Jack/SoPlex: 99.81 2nd place
 - SCIP-Jack/CPLEX: 100



Prize-collecting Steiner tree problem



Prize-Collecting Steiner Trees

Given:

- ▷ undirected graph G = (V, E)
- \triangleright vertex costs $p \in \mathbb{R}_{\geq 0}^V$
- \triangleright edge costs $c \in \mathbb{R}_{\geq 0}^{E}$

Prize-Collecting Steiner Tree Problem (PCSTP)

Find a tree $S \subseteq G$ such that

 $\triangleright \sum_{e \in E(S)} c(e) + \sum_{v \in V \setminus V(S)} p(v)$ is minimized

 $T_{p} := \{v \in V \mid p(v) > 0\}$ are called potential terminals.

Transformation: PCSPG to SAP



Transformation to SAP ...

- $\triangleright\,$ allows to use powerful cut-separation routine of SCIP-Jack
- $\triangleright\,$ allows to employ strong heuristics based on a dual-ascent algorithm for SAP

Transformation: PCSPG to SAP



Transformation to SAP ...

- $\triangleright\,$ allows to use powerful cut-separation routine of SCIP-Jack
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works, but not enough to be competitive...

Reduction techniques

Some recent work ...

Definition

Let $v_i, v_j \in V$. Call walk $W = (v_{i_1}, e_{i_1}, v_{i_2}, e_{i_2}, ..., e_{i_r}, v_{i_r})$ with $v_{i_1} = v_i$ and $v_{i_r} = v_j$ prize-constrained (v_i, v_j) -walk if no $v \in T_p \cup \{v_i, v_j\}$ contained more than once in W.

Definition

Define *prize-collecting cost* of W as

$$c_{pc}(W) := \sum_{e \in E(W)} c(e) - \sum_{v \in V(W) \setminus \{v_i, v_j\}} p(v).$$

Definition

Define *prize-constrained length* of W:

 $I_{pc}(W) := \max\{c_{pc}(W(v_{i_k},v_{i_l})) \mid 1 \leqslant k \leqslant l \leqslant r, \ v_{i_k}, v_{i_l} \in T_p \cup \{v_i,v_j\}\}.$

Let $\mathcal{W}_{pc}(v_i, v_j)$ prize-constrained (v_i, v_j) -walks define *prize-constrained* distance between v_i and v_j :

$$d_{pc}(v_i, v_j) := \min\{I_{pc}(W') \mid W' \in \mathcal{W}_{pc}(v_i, v_j)\}.$$

Proposition

Let $\{v_i, v_j\} \in E$. If

$$c(\{v_i, v_j\}) > d_{pc}(v_i, v_j)$$

is satisfied, then $\{v_i, v_j\}$ cannot be contained in any optimal solution.

Prize-constrained concept allows for very powerful reduction tests; dominates previous concept from Uchoa 2006 (Oper. Res. Let.) and generalizes tests known for SPG.

Downside: NP-hard. But: Nice (easy to implement) approximation by an extension of Dijkstra's algorithm.

Prize-constrained walks (2)

Another use of prize-constrained walks:

Definition

Let W be prize-constrained (v_i, v_j) walk. Define *left-rooted* prize-constrained length of W as:

$$I_{pc}^{-}(W) := \max\{c_{pc}(W(v_i, v_{i_k})) \mid v_{i_k} \in V(W) \cap (T_p \cup \{v_j\})\}.$$

Definition

Define *left-rooted prize-constrained* (v_i, v_j) -*distance* as:

$$d^-_{pc}(v_i, v_j) := \min\{I^-_{pc}(W') \mid W' \in \mathcal{W}_{pc}(v_i, v_j)\}.$$

Proposition

Let $v_i, v_i \in V$. If

$$p(v_i) > d^-_{pc}(v_i, v_j),$$

then every optimal solution that contains v_i also contains v_i .

Using left-rooted prize-constrained walks



- ▷ Use prize-constrained walks to identify terminals t_i that need to be part of all optimal solutions
- ▷ ...allows for better transformation to SAP:

INPUT: RPCSTP (V, E, T_f , c, p) and t_p , $t_q \in T_f$ $T_f := \{t_1, t_2, ..., t_z\}$ fixed terminals OUTPUT: SAP

- 1. Set V' := V, $A' := \{(v, w) \in V' \times V' \mid \{v, w\} \in E\}$, c' := c, $r' := t_q$.
- 2. For each $i \in \{1, ..., z\}$: 2.1 add node t'_i to V', 2.2 add arc (t_i, t'_i) of weight 0 to A', 2.3 add arc (t_p, t'_i) of weight $p(t_i)$ to A'.
- 3. Define set of terminals $T' := \{t'_1, ..., t'_z\} \cup T_f$.
- 4. **Return** (V', A', T', c', r').



We have recently proved: Choice of t_p , t_q does not change LP value! But: Can have strong impact in practival solving, natural candidate for UG racing ramp up parameter!

Prize-constrained walks in branch-and-cut

- > preprocessing
- ▷ probing
- > propagation
- ▷ cutting planes
- primal heuristics
- b dual heuristics
- ⊳ B&B

We can exploit that when using UG!

Performance of SCIP-Jack on PCSTP

Many PCSTP solvers introduced in the literature lately, the two best:

- ▷ Fischetti et. al. 2017 (Math. Prog. C)
- ▷ Leitner et. al. 2018 (INFORMS J. Comput.) ... stronger by far

		mean	time [s]	max. 1	time [s]	# solved	
Test set	#	L18	SJ	L18	SJ	L18	SJ
JMP	34	0.0	0.0	0.0	0.0	34	34
Cologne1	14	0.0	0.0	0.1	0.0	14	14
Cologne2	15	0.1	0.1	0.2	0.1	15	15
CRR	80	0.1	0.1	5.7	1.1	80	80
ACTMOD	8	0.9	0.3	3.5	1.5	8	8
E	40	1.8	0.2	>3600	34.5	37	40
HANDBI	14	36.5	14.9	>3600	>3600	12	13
HANDBD	14	34.1	13.3	>3600	>3600	13	13
1640	100	8.7	6.1	>3600	>3600	90	91
PUCNU	18	278.9	80.2	>3600	>3600	7	11
Н	14	488.7	477.4	>3600	>3600	4	5
			SJ - SCIF	P-Jack			
		L18 -	Leitner e	et. al. 201	18		

- SCIP-Jack often more than two or three orders of magnitude faster than next best solver (from Fischetti et. al. 2017, Math. Prog. C).
 E.g. max. time on Cologne2:
 - Fischetti et. al.: > 200 seconds
 - ► SCIP-Jack: < 0.1 seconds
- Recent PCSTP improvements of SCIP-Jack allowed us to solve two and improve best known solutions for more than one third of unsolved DIMACS 2014 instances.

Parallelization of SCIP-Jack by UG

- ▷ UG framework to parallelize B&B search both in shared, ug[SCIP-Jack, C++11 threads], and distributed, ug[SCIP-Jack, MPI], environments.
- ▷ Parallelization can be realized with a few lines of code.
- ▷ ... but to improve performance both UG and SCIP-Jack had to be extended.
- Difficulties:
 - Long running time in root node.
 - Special branching.
 - Distributing problem specific preprocessing effects.

SCIP-Jack branches on vertices of the graph. Including vertex *v* corresponds to the constraint:

$$\sum_{a\in\delta^-(v)}x_a=1$$

Excluding vertex v corresponds to constraint:

$$\sum_{a\in\delta^-(v)\cup\delta^+(v)}x_a=0$$

added new features to UG to allow branching on constraints
 ...but (in particular for PCSTP) we need to adapt underlying graph!

- SCIP-Jack/UG transfers branching history together with subproblem. SCIP-Jack changes underlying graph (e.g. deletes vertices).
- Improves finding locally valid solutions and helps cut generation.
 Local cuts also transferred by UG.
- Using branching history for separation and heuristics, we got speed-up of about 30% with 32 threads.

Strong point of UG: presolving of subproblems during branch-and-bound.

Problem:

- ▷ For Steiner tree problems MIP presolving remarkably unsuccessful.
- Complex Steiner reduction techniques not easy to reflect in IP. Thus Steiner tree solvers only perform reductions to delete vertices and edges during B&B.

We make use of following observation:

Aggressive presolving of subproblems(2)

Each SCIP-Jack Steiner tree reduction transforms SPG (V, E, T, c) to SPG (V', E', T', c') and provides function $p : E' \to \mathcal{P}(E)$ such that for each (optimal) solution $S' \subseteq E'$ to transformed problem, set $\bigcup_{e \in S'} p(e)$ is (optimal) solution to original problem.

Observation

Let (V, E, T, c), (V', E', T', c'), and p as above. Define $E'' := \bigcup_{e \in E'} p(e)$, $V'' := \{v \in V \mid \exists (v, w) \in E'', w \in V\}$, $T'' := \{t \in T \mid \exists (t, w) \in E'', w \in V\}$, $c'' := c|_{E''}$. Each (optimal) solution to (V'', E'', T'', c'') is (optimal) solution to (V, E, T, c). Observation allows us to perform aggressive presolving whenever new subproblems are initialized. About 25% speed-up with 32 threads and improved scaling behaviour.

Racing ramp-up with customized racing paramaters (new feature of UG) is also used.

Shared memory results for PCSTP

Threads	i640-115	i640-141	cc10-2nu	cc7nu				
1	201	809	812	4,333				
8	102	314	311	1,922				
16	80	210	200	1,023				
32	78	110	167	843				
64	79	101	165	723				
root time	15	28	107	55				
$\max \#$ solvers	13	48	34	64				
first max active time	55	152	211	301				
All times in seconds								

We performed experiments on PUC, the most difficult Steiner tree test set: 29 of 50 instances have remained unsolved.

SCIP-Jack (sequential) is currently the strongest solver on PUC:

- \triangleright # instances solved in one hour:
 - ▶ 13 by SCIP-Jack:
 - 12 by best other (Polzin, Vahdati Daneshmand, 2014)¹
- $\triangleright~\#$ instances solved in 12 hours:
 - ▶ 18 by SCIP-Jack:
 - ▶ 13 by best other (Polzin, Vahdati Daneshmand, 2014)

²Run time is scaled, as solver is not publicly available

- Two years ago on the PUC test set ug[SCIP-Jack, MPI]:
- ▷ improved primal bounds for 14 instances
- ▷ solved three instances to optimality for first time

In recent computational experiments we were able to

- ▷ improve two best known primal bounds
- $\triangleright\,$ solve one previously unsolved instance

Solving hc9p

Table 1: Statistics for so	lving hc9p on	supercomputers
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Dun	Computer	Caraa	Time	Idle	Trong	Primal bound	Dual bound	Gap	Nodas	Onen nodes	
Kun Computer Co		Coles	(sec.)	(%)	Trans.	(Upper bound)	(Lower bound)	(%)	Inodes	Open nodes	
1	ISM	72	604,796	< 0.3	738	30,242.0000	29,879.3721	1.21	0	0	
1	131/1	12	(317)	0.5	150	30,242.0000	30,058.9366	0.61	110,012,624	1,257,112	
2 ISM	IGM	2,304	604 704	< 1.5	< 1.5	070 605	30,242.0000	30,058.7930	0.61	0	15
	131/1		004,794		979,095	30,242.0000	30,102.7556	0.46	3,758,532,600	723,167	
2	2 HI DN III 24 574	24 576	1 576 86 336	6 < 17	8 811 512	30,242.0000	30,102.6645	0.46	0	35	
J ILKN III	24,570	10 00,550	1 .7	0,011,012	30,242.0000	30,116.3592	0.42	2,402,406,311	575,678		
4 HLRN	III DN III	I 12,288	42 100	< 1.5	< 1.5	1 700 027	30,242.0000	30,115.3331	0.42	0	3,709
	HLKN III		12,200 43,15	45,199		1,709,027	30,242.0000	30,120.4801	0.40	664,909,985	602,323
5 III DN III	12 200	12 289 119 250	1.5	0.159.020	30,242.0000	30,120.4801	0.40	0	285		
3	ILKN III	12,200	110,239	1.5	9,158,920	30,242.0000	30,242.0000	0.00	1,677,724,126	0	

Supercomputers used:

- ISM: HPE SGI 8600 with 384 compute nodes, each node has two Intel Xeon Gold 6154 3.0GHz CPUs(18 cores×2) sharing 384GB of memory, and Infiniband (Enhanced Hypercube) interconnect
- HLRN III: Cray XC40 with 1872 compute nodes, each node with two 12-core Intel Xeon Ivy- Bridge/Haswell CPUs sharing 64 GiB of RAM, and with Aries interconnect

How open nodes and active solvers evolved (hc9p)



Figure 1: Evolution of computation for solving hc9p by using 12,288 cores (Run 5)

Solving hc11p

Run Computer	Coras	Time	Idle	Trong	Primal bound	Dual bound	Gap	Nodes	Onen nodes	
	Computer	Cores	(sec.)	(%)	frans.	(Upper bound)	(Lower bound)	(%)	induces	Open nodes
1.1	ISM	72	604,799	< 0.3	71	119,492.0000	117,388.8528	1.79	0	0
1.1 15101	131/1	12	(2,558)	< 0.5	/1	119,297.0000	117,496.5470	1.53	4,314,198	1,109,629
1.2		12 299	43,149	< 0.5	21 204	119,297.0000	117,388.7971	1.63	0	0
1.2 ILKN III	12,200	(7,164)	< 0.5 51,504	119,297.0000	117,426.2226	1.59	28,491,470	5,433,482		
2	2 HLRN III 43,000	I DN III 42 000 86 354	< 1.0	96 152	119,297.0000	117,426.2226	1.59	0	103	
		45,000	00,554	< 4.9	00,152	119,297.0000	117,468.8459	1.56	267,513,609	40,499,188

 Table 2: Statistics for solving hcllp on supercomputers

Supercomputers used:

- ISM: HPE SGI 8600 with 384 compute nodes, each node has two Intel Xeon Gold 6154 3.0GHz CPUs(18 cores×2) sharing 384GB of memory, and Infiniband (Enhanced Hypercube) interconnect
- HLRN III: Cray XC40 with 1872 compute nodes, each node with two 12-core Intel Xeon Ivy- Bridge/Haswell CPUs sharing 64 GiB of RAM, and with Aries interconnect

How open nodes and active solvers evolved (hc11p)



Figure 2: Evolution of computation for solving hcllp by using 43,000 cores (Run 2)

We plan to

- ▷ (considerably) improve sequential performance of both SPG and related problems
- ▷ add internal shared memory parallelizations to SCIP-Jack And:
- ▷ solve more open PUC instances with ug[SCIP-Jack, MPI]
- ▷ solve open instances of related problems with ug[SCIP-Jack, MPI]

We plan to

- ▷ (considerably) improve sequential performance of both SPG and related problems
- ▷ add internal shared memory parallelizations to SCIP-Jack And:
- ▷ solve more open PUC instances with ug[SCIP-Jack, MPI]
- ▷ solve open instances of related problems with ug[SCIP-Jack, MPI]

Thank you!

Some references

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SCIP Opt. Suite: http://scip.zib.de