Probabilistic Subproblem Selection in Branch–and–Bound Algorithms

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General B&B Framework (1)

Problem:

$$\max f(x) \quad \text{s.t. } x \in \mathcal{M}.$$

Step 0. Compute a compact set $X \supset \mathcal{M}$ of simple structure. Compute an upper bound $u(X) \geq \max_{x\in\mathcal{M}} f(x)$, as well as a lower bound $\ell(X) \leq \max_{x\in\mathcal{M}} f(x)$.
Let $\mathcal{L}$ be an empty list, and set $k := 1$.

Step 1. Partition X into ν compact subsets $X_1, \ldots, X_\nu$, and add them to the list $\mathcal{L}$.

Step 2. Calculate upper bounds $u(X_i) \geq \max_{x\in X_i\cap\mathcal{M}} f(x)$ and lower bounds $\ell(X_i) \leq \max_{x\in X_i\cap\mathcal{M}} f(x)$ for all new sets X_i.

General B&B Framework (2)

Step 3. Update the current best upper and lower bounds: Put

$$u_k := \max_{X \in \mathcal{L}} u(X) \qquad \text{and} \qquad \ell_k := \max_{X \in \mathcal{L}} \ell(X).$$

Step 4. Discard elements from $\mathcal{L}$ which can not contain a global optimizer, i.e. discard all elements X with the property (i) $X \cap \mathcal{M} = \emptyset$, or (ii) $u(X) < \ell_k$.

Step 5. **Select a new $X \in \mathcal{L}$ which is to be subdivided in the next iteration**, and remove it from $\mathcal{L}$.

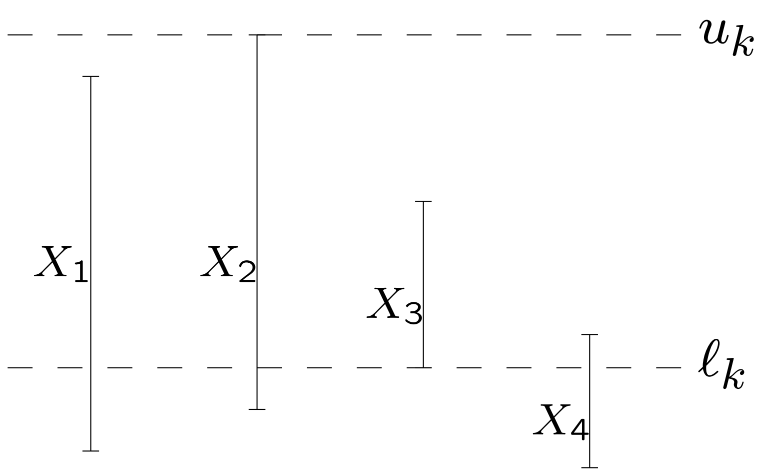
Step 6. While stopping criteria are not fulfilled, increment $k := k + 1$, and go to Step 1.

Possible Selection Rules (1)

Traditional Rule:

Select the dominating set $\overline{X}$ (i.e. the set with the highest upper bound $u(X)$).

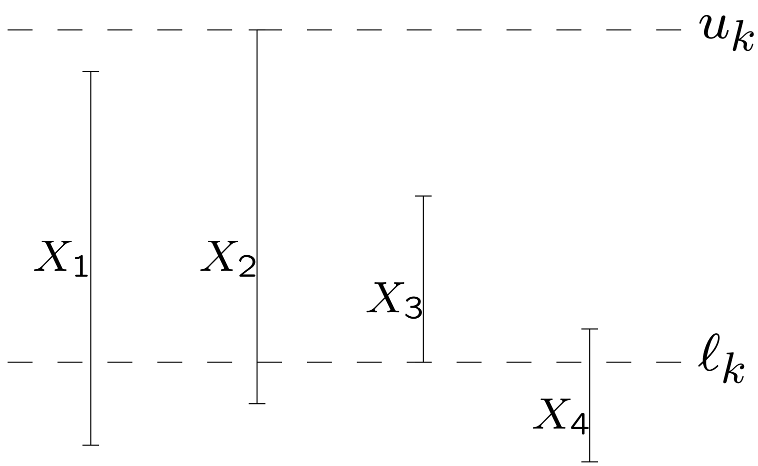
Convergence: guaranteed.



Possible Selection Rules (2)

Stix' Rule:

Select all sets whose upper bound exceeds a certain target value: $u(X) \geq \tau$.



Convergence: guaranteed.

Performance: improved.

Possible Selection Rules (3)

Csendes' Rule:

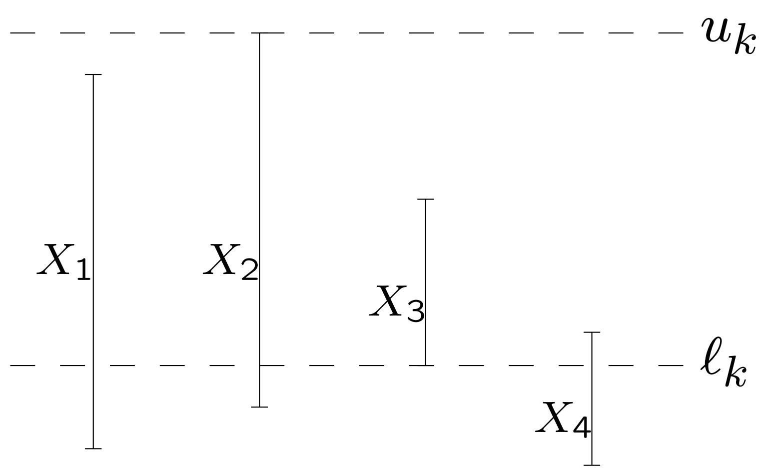
Select the set for which

$$I(X) = \frac{u(X) - \max_{x \in \mathcal{M}} f(x)}{u(X) - \ell(X)}$$

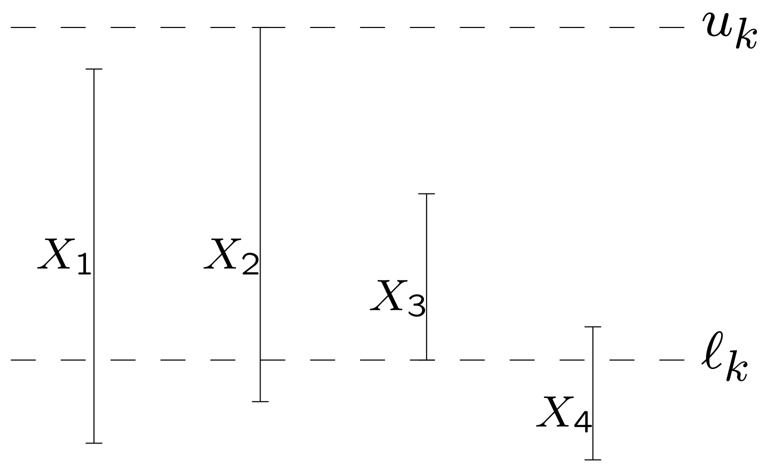
is maximized.

Convergence:
not guaranteed.

Performance: very good.



Idea: Probabilistic Selection Rule



Some sets "more likely" to contain global solution than others.

Therefore: select according to a probability distribution!

$$\boldsymbol{P}_k(X_i \text{ is selected in iteration } k) \propto \frac{u(X_i) - \ell_k}{u_k - \ell_k}.$$

Some Definitions

Definition 1:

A partitioning procedure is called exhaustive, if every nested sequence $\{X_i\}_{i\in\mathbb{N}}$ of partition sets eventually shrinks to a singleton:

$$\bigcap_{i\in\mathbb{N}} X_i = \{x^*\}.$$

Definition 2:

We say that a bounding procedure has the zero convergence property, if for every exhaustive sequence $\{X_i\}_{i\in\mathbb{N}}$ of subsets of X_0 we have

$$\lim_{i\to\infty} u(X_i) = \lim_{i\to\infty} \ell(X_i).$$

Convergence of B&B

Proposition:

Assume that in a Branch–and–Bound procedure

(a) a selection rule is used which ensures that the dominating set is chosen infinitely often,

(b) an exhaustive partitioning procedure is used, and

(c) the bounding procedure has the zero convergence property.

Then the B&B procedure is convergent, i.e.

$$\lim_{k\to\infty} u_k = \lim_{k\to\infty} \ell_k.$$

Convergence of B&B with Probabilistic Selection Rule

Theorem:

Assume that in a Branch–and–Bound procedure

(a) a probabilistic selection rule is used which fulfills

$$\sum_{k=0}^{\infty} \boldsymbol{P}_k(\overline{X}_k \text{ is selected in iteration } k) = +\infty,$$

(b) an exhaustive partitioning procedure is used, and

(c) the bounding procedure has the zero convergence property.

Then the B&B procedure converges with probability 1.

Which probabilistic selection rules fulfill convergence conditions? (1)

$$\boldsymbol{P}_k(X_i \text{ is selected in iteration } k) = \frac{u(X_i) - \ell_k}{\sum_{X \in \mathcal{L}_k} (u(X) - \ell_k)}.$$

The dominating set is assigned the highest probability among all $X \in \mathcal{L}_k$, and $|\mathcal{L}_k| \le k\nu$.

$$\boldsymbol{P}_k(\overline{X}_k \text{ is selected in iteration } k) \ge \frac{1}{k\nu}.$$

Therefore:

$$\sum_{k=0}^{\infty} \boldsymbol{P}_k(\overline{X}_k \text{ is selected in iteration } k) \ge \frac{1}{\nu} \sum_{k=0}^{\infty} \frac{1}{k} = +\infty.$$

Which probabilistic selection rules fulfill convergence conditions? (2)

Theorem:

Assume that in a Branch–and–Bound procedure

(a) a selection rule is used which ensures that in each iteration the dominating set is assigned the highest probability among all elements of the list,

(b) the number of elements in the list increases at most linearly in the iterations,

(c) an exhaustive partitioning procedure is used, and

(d) the bounding procedure has the zero convergence property.

Then the B&B procedure is convergent with probability 1.

Which probabilistic selection rules fulfill convergence conditions? (3)

Other possibility:

$$\boldsymbol{P}'_k(X_i \text{ is selected in iteration } k) = \frac{F\left(\frac{u(X_i)-\ell_k}{u_k-\ell_k}\right)}{\sum\limits_{X\in\mathcal{L}_k} F\left(\frac{u(X)-\ell_k}{u_k-\ell_k}\right)},$$

where F is any probability distribution function on $[0,1]$.

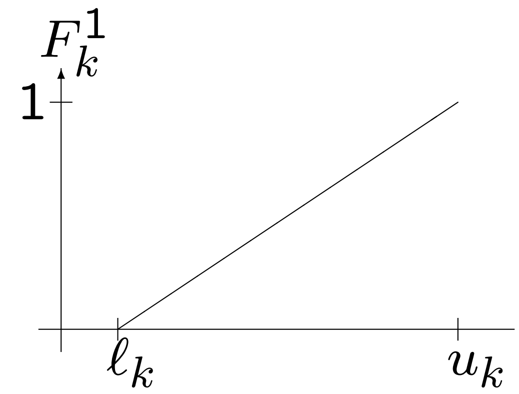
Order of probabilities of the sets does not change:

$$\boldsymbol{P}_k(X_i) \le \boldsymbol{P}_k(X_j) \quad \Longleftrightarrow \quad \boldsymbol{P}'_k(X_i) \le \boldsymbol{P}'_k(X_j).$$

$\Rightarrow$ Convergence conditions fulfilled.

Special Instances of F (1)

Uniform distribution:

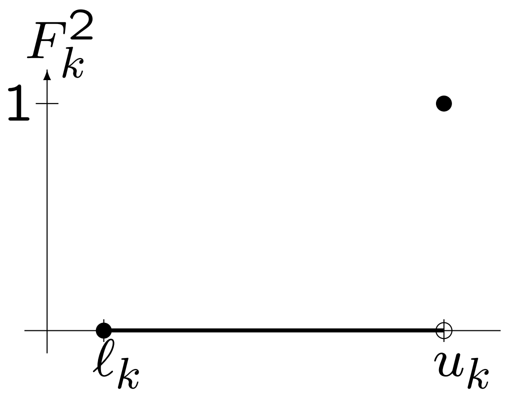


yields our original probability measure:

$$\boldsymbol{P}_k(X_i \text{ is selected in iteration } k) = \frac{u(X_i) - \ell_k}{\sum_{X \in \mathcal{L}_k} (u(X) - \ell_k)}.$$

Special Instances of F (2)

Distribution F^2:



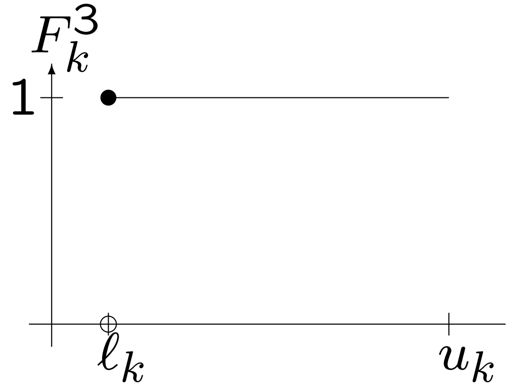
$$F^2(x) = \begin{cases} 0 & \ldots & 0 \le x < 1 \\ 1 & \ldots & x = 1 \end{cases}$$

yields the purely deterministic selection rule:

Always select the set with the highest upper bound.

Special Instances of F (3)

Distribution F^3:



$$F^3(x) = 1 \quad \text{for} \quad 0 \le x \le 1.$$

yields the purely random selection rule:

$$\boldsymbol{P}_k^3(X_i \text{ is selected in iteration } k) = \frac{1}{\sum_{X \in \mathcal{L}} 1} = \frac{1}{|\mathcal{L}|},$$

Numerical Tests on Maximum Clique Problem

Reformulation:

$$\begin{aligned} &\max x^T A_{\mathcal{G}} x \\ &\text{s.t. } x \in \Delta \end{aligned} \qquad (\star)$$

where: $A_{\mathcal{G}}$ is regularization of adjacency matrix – indefinite!!
Δ is the standard simplex.

Theorem (I.M.Bomze):

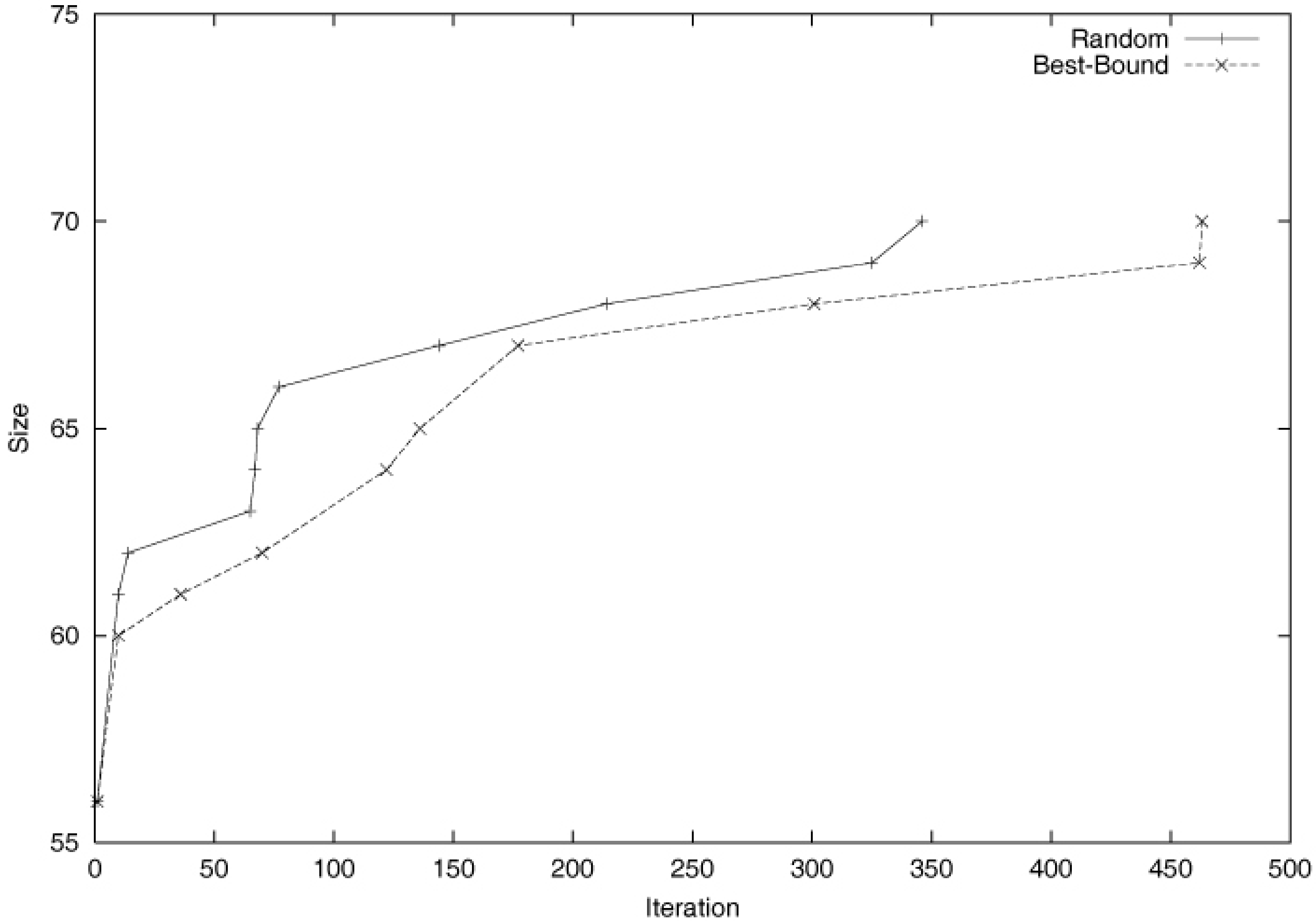
There is a one to one correspondance between:

1.) local solutions of $(\star)$ and maximal cliques,

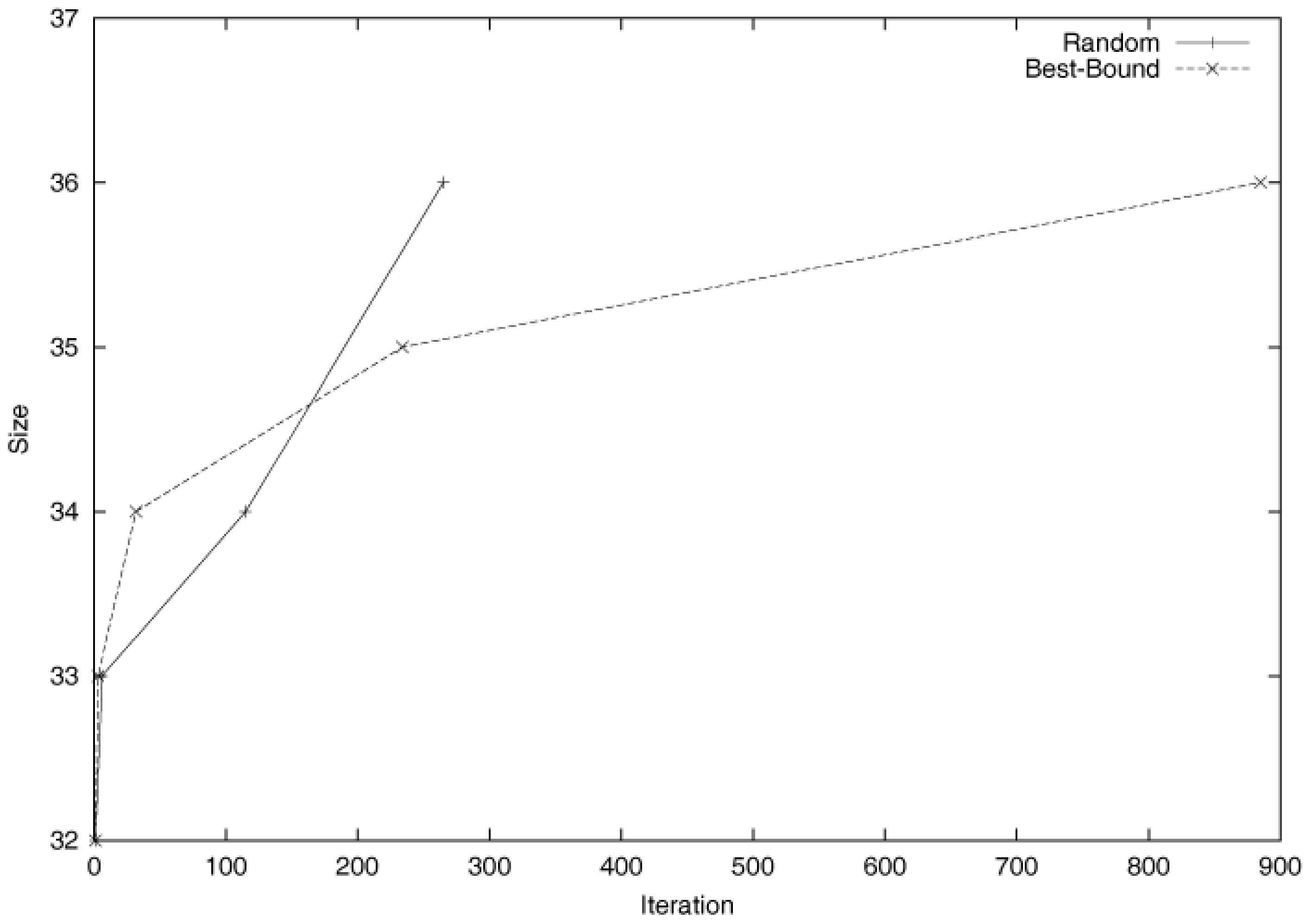
2.) global solutions of $(\star)$ and maximum cliques.

We used DIMACS benchmark graphs as testproblems.

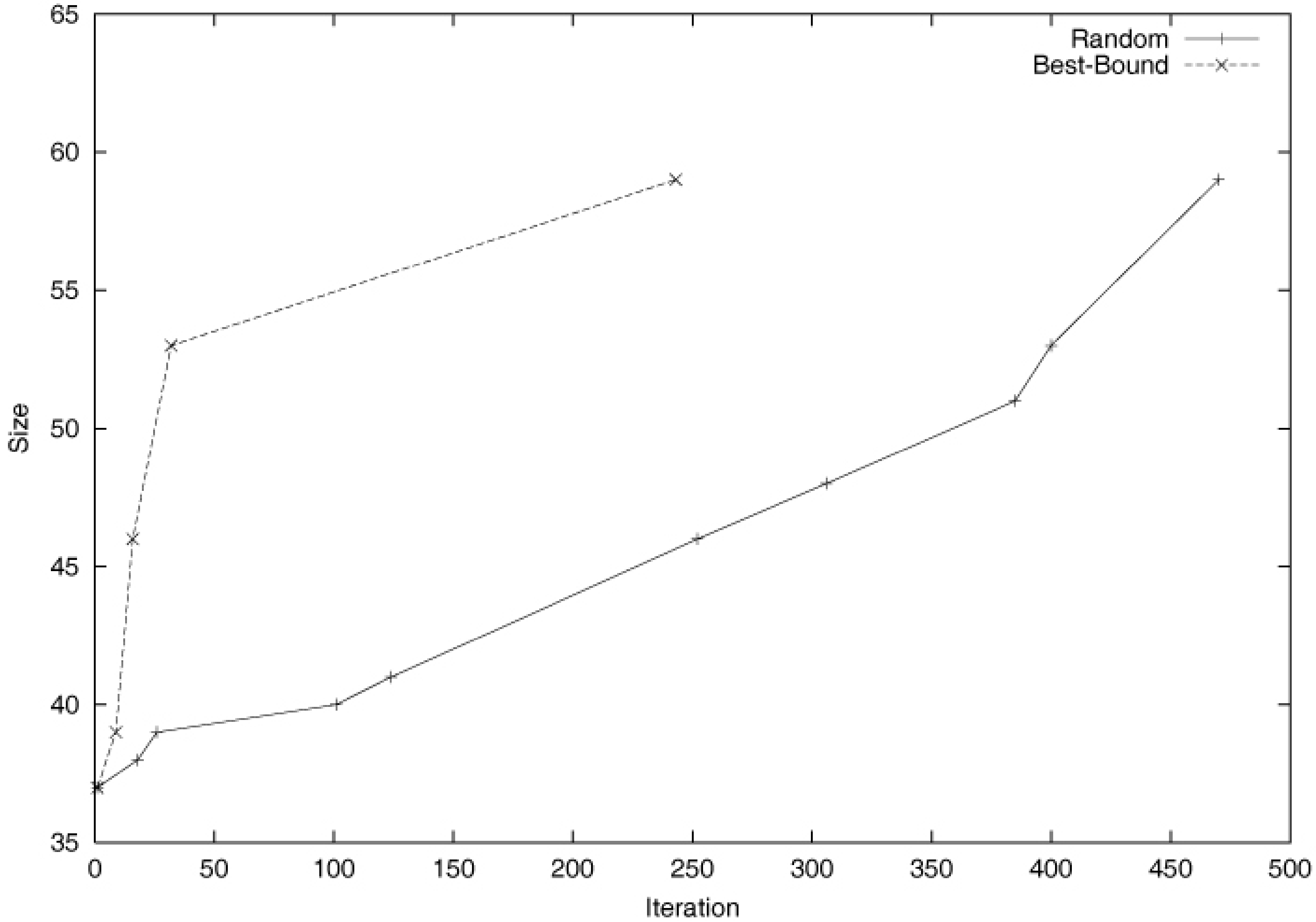
Performance: `san200_0.9_1`



Performance: `san200_0.9_3`



Performance: `san200_0.9_2`



Experiments on DIMACS Graphs:

name	dimension	random			best	performance
		min.	avg.	max.	bound	
brock200_1	200	**1497**	**1935.45**	**2103**	2802	69%
brock400_1	400	**25**	**72.85**	**102**	105	69%
brock400_2	400	**17**	**67.20**	107	90	71%
brock400_3	400	**41**	163.45	259	99	165%
brock400_4	400	**8**	**254.45**	560	330	77%
MANN_a27	378	**9**	**16.25**	**30**	123	13%
p_hat300-2	300	**2833**	4603.75	5079	3628	127%
p_hat300-3	300	**53**	**145.10**	288	156	93%
san200_0.9_2	200	**136**	253.90	348	243	104%
san200_0.9_3	200	**92**	**853.2**	1732	885	96%
san400_0.7_1	400	**23**	142.30	207	88	162%
san400_0.7_2	400	**688**	**1046.60**	**1865**	2777	38%
san400_0.7_3	400	**38**	833.70	1291	462	181%
san400_0.9_1	400	**18**	**192.10**	511	272	71%
sanr200_0.7	200	**12**	**77.25**	**132**	144	53%
sanr200_0.9	200	**694**	**3468.05**	8613	3512	98%
sanr400_0.7	400	**44**	**216.90**	372	257	84%