Computer science

— Theory vs Experimentation —

Part 3: Algorithm Engineering

Christine Solnon

INSA de Lyon - 5IF

2023 / 2024

In almost every computation, a great variety of arrangements for the succession of the processes is possible, and various considerations must influence the selection amongst them for the purposes of a Calculating Engine. One essential object is to choose that arrangement which shall tend to reduce to a minimum the time necessary for completing the calculation.

Ada Byron, 1843

3 possible levels of tuning:

- Algorithm $\rightsquigarrow$ Divide-and-conquer, Dynamic Programming, ...
- Code $\rightsquigarrow$ Loops, Memory management, ...
- Parameters $\rightsquigarrow$ Best setting for each instance / class of instances

Goal:

- Improve performance (time, memory consumption, ...)
- In most cases, theoretical complexities are not changed
  But empirical performance may be greatly improved!

Plan

Some General Rules to Improve Algorithms

Use memory to save time

- Memoize sub-problem solutions (dynamic programming)
- Incrementally maintain data instead of recomputing it from scratch
- etc...

Use relevant data structures

- Study operation frequencies to choose the best data structure
  $\leadsto$ Hash table, Tree, Heap, Disjoint-sets, Sparse-sets, Dancing links, . . .

Exit from loops as soon as possible

Examples: Dijkstra, Bellman-Ford, . . .

Prune branches of search trees

- Compute tight bounds on objective functions $\leadsto$ Branch & Bound
- Propagate constraints $\leadsto$ Branch & Propagate

Illustration on the TSP

Permut: Enumate all permutations $\rightsquigarrow \mathcal{O}(n!)$

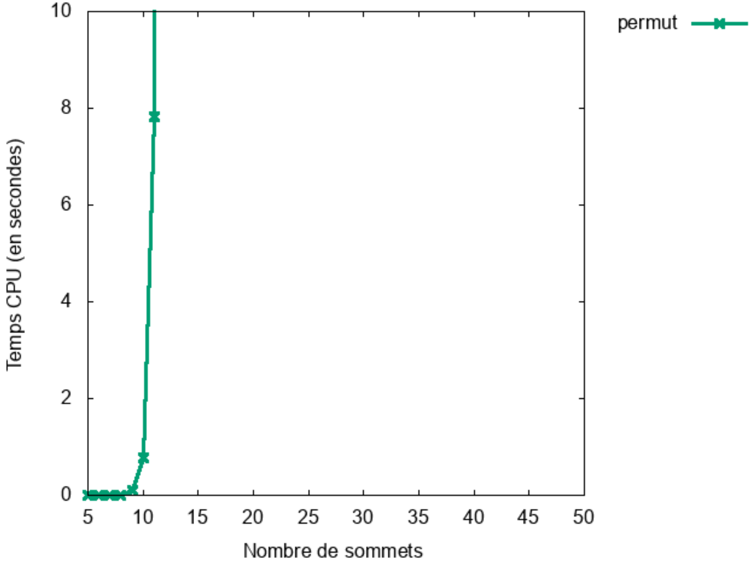


Illustration on the TSP

Stop: Prune the current branch if current length $\geq$ best

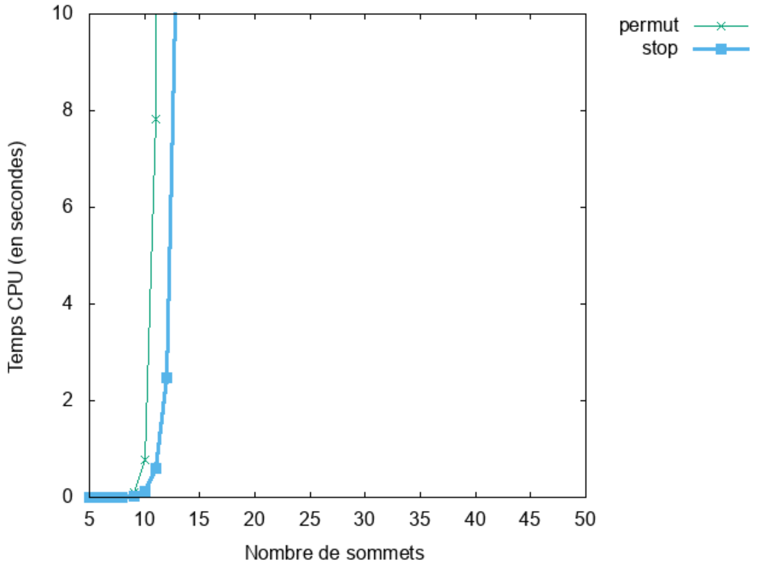


Illustration on the TSP

Branch & Bound 1: Bound = $d_{min} * nbNotVisited$

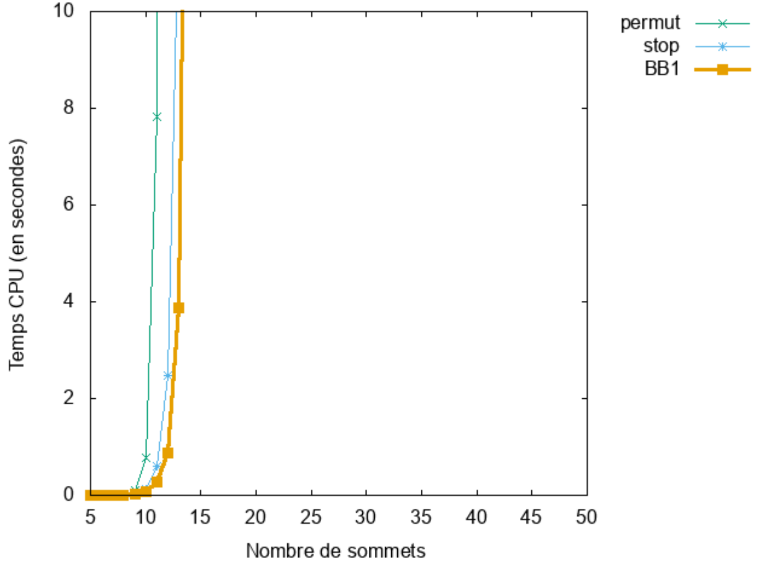


Illustration on the TSP

Branch & Bound 2: Bound = $\sum_{i \in notVisited} \min_{j \in notVisited, j \neq i} d_{ij}$

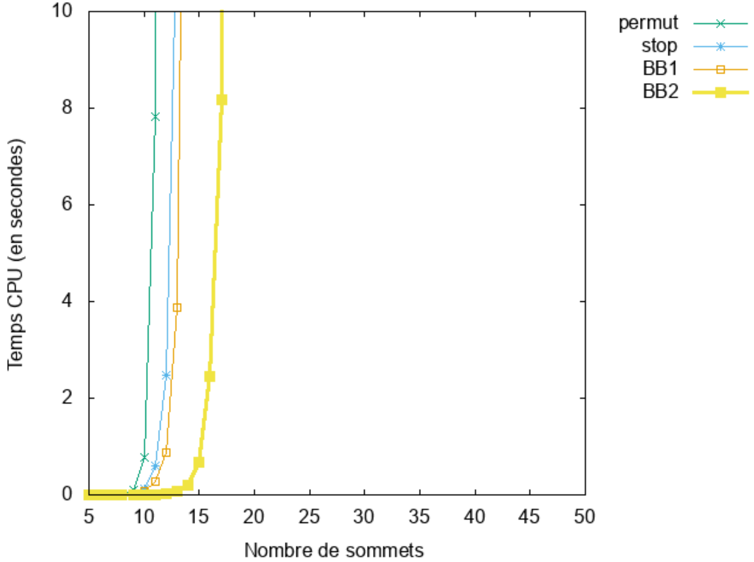


Illustration on the TSP

Branch & Bound 3: Bound = minimal 1-tree cost

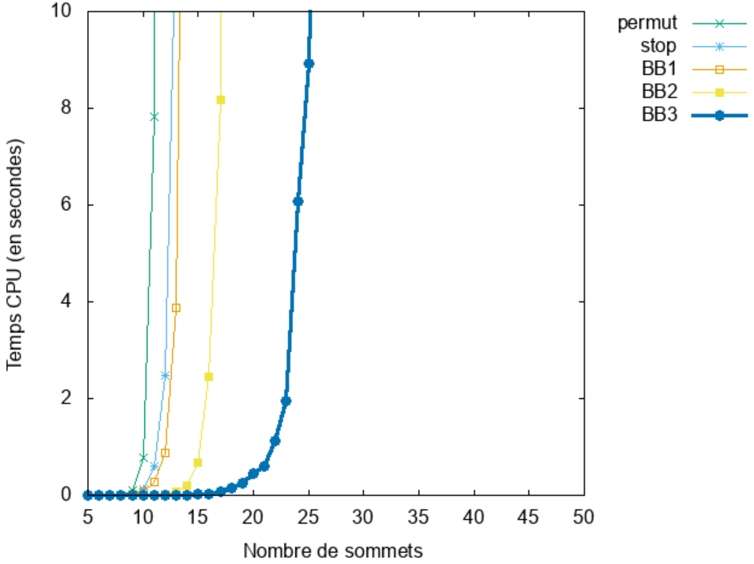


Illustration on the TSP

Branch & Bound 4: Bound = subgradian opt. of Held-Karp (iterated 1-tree)

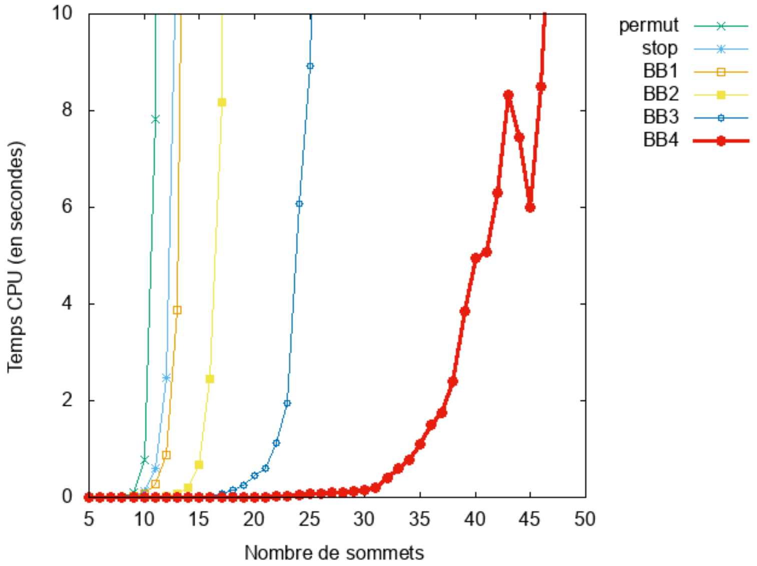


Illustration on the TSP

Branch & Bound 4 + h: Addition of an ordering heuristic

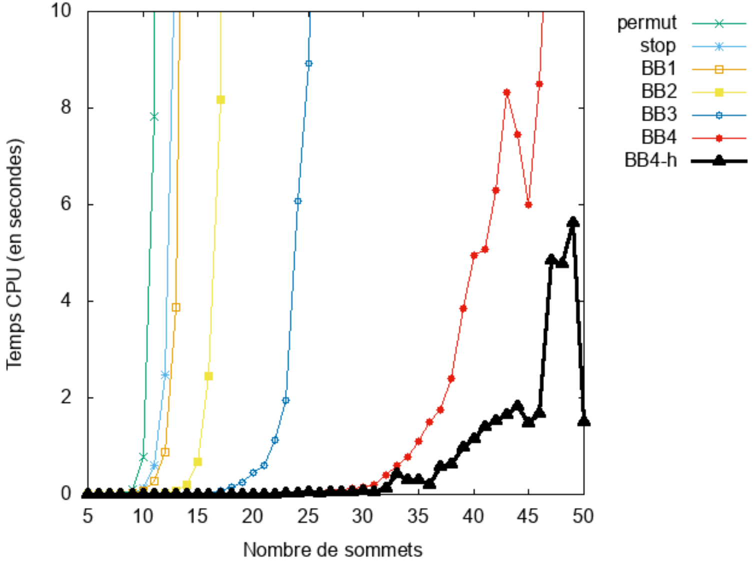


Illustration on the TSP

DPrec: Recursive Dynamic Programming $\rightsquigarrow \mathcal{O}(n^2 \cdot 2^n)$

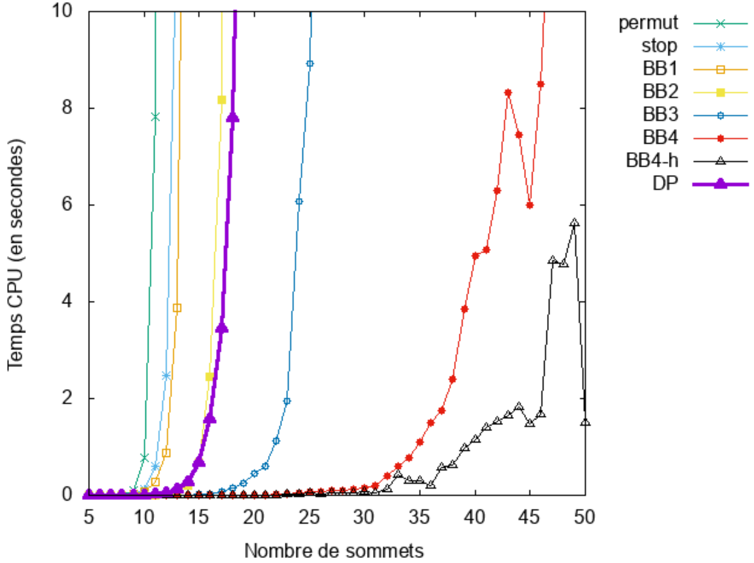


Illustration on the TSP

DPiter: Iterative Dynamic Programming $\rightsquigarrow \mathcal{O}(n^2 \cdot 2^n)$

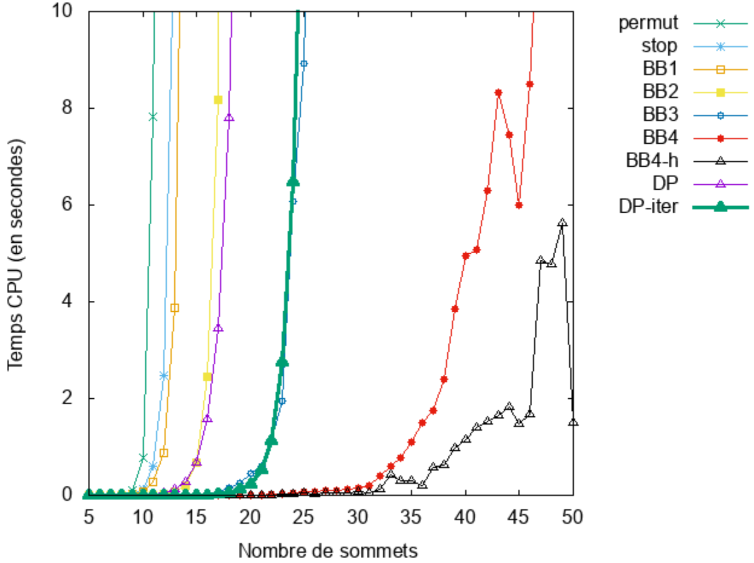


Illustration on the TSP

What if we change the benchmark?

Model used to generate graphs in the previous slide:

- Random generation of n coordinates $(x, y) \in [0, 1000]^2$
  $\rightsquigarrow$ Uniform distribution
- Edge cost = Euclidean distance (rounded to the closest integer value)

$\rightsquigarrow$ Experiments on 10 graphs (performance measure = average CPU time)

New model:

- For each edge: random generation of an integer cost $\in [10, 20]$
  $\rightsquigarrow$ Uniform distribution

$\rightsquigarrow$ Experiments on 10 graphs (performance measure = average CPU time)

Illustration on the TSP

What if we change the benchmark?

Model used to generate graphs in the previous slide:

- Random generation of n coordinates $(x, y) \in [0, 1000]^2$
  $\rightsquigarrow$ Uniform distribution
- Edge cost = Euclidean distance (rounded to the closest integer value)

$\rightsquigarrow$ Experiments on 10 graphs (performance measure = average CPU time)

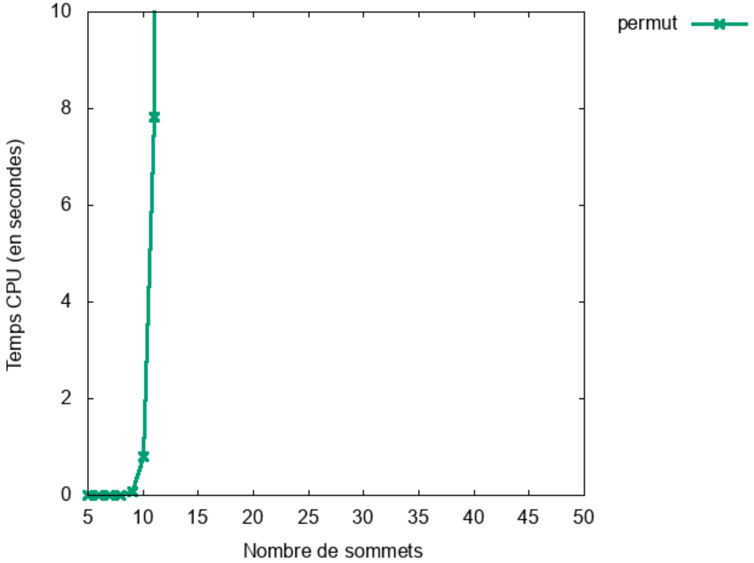
New model:

- For each edge: random generation of an integer cost $\in [10, 20]$
  $\rightsquigarrow$ Uniform distribution

$\rightsquigarrow$ Experiments on 10 graphs (performance measure = average CPU time)

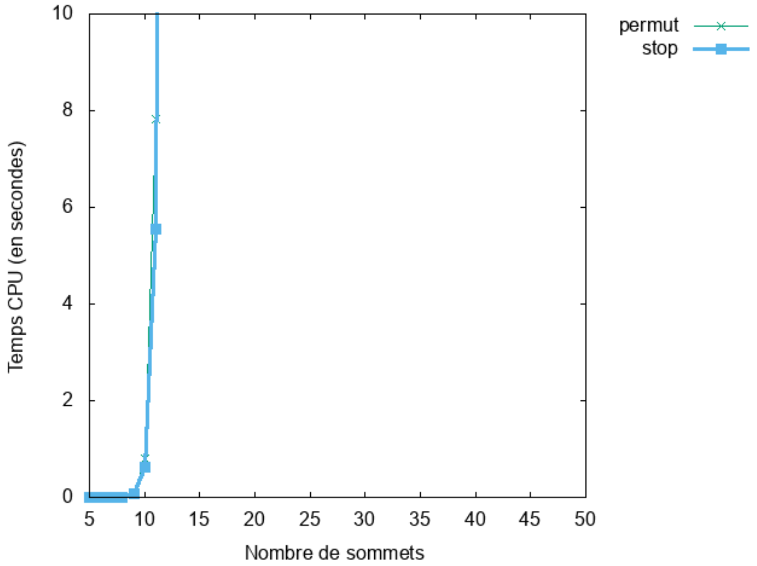
Results on Benchmark 2

Permut: Enumate all permutations $\rightsquigarrow \mathcal{O}(n!)$



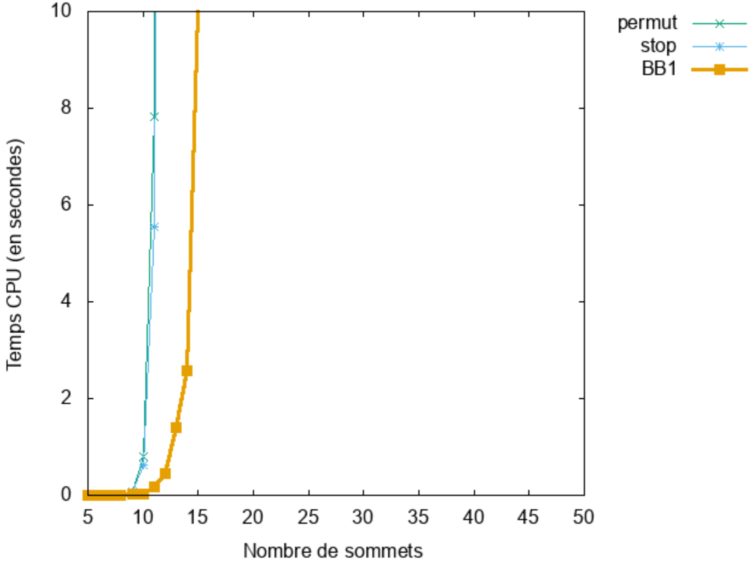
Results on Benchmark 2

Stop: Prune the current branch if current length $\geq$ best



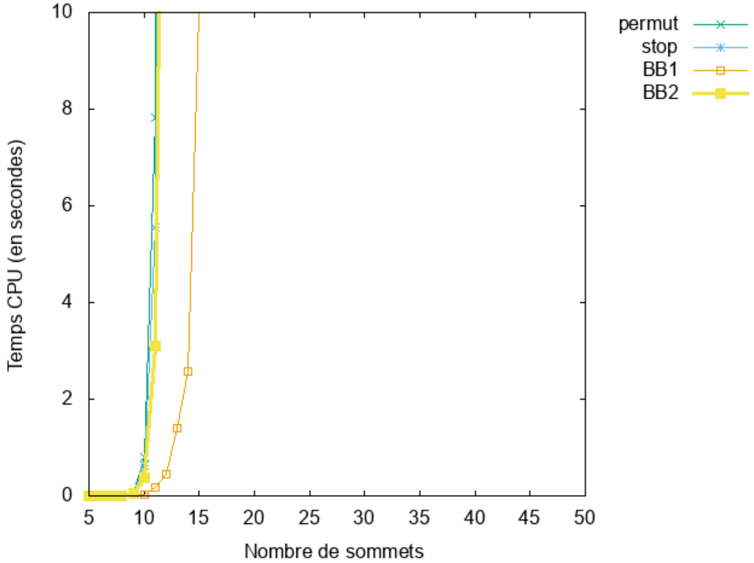
Results on Benchmark 2

Branch & Bound 1: Bound = $d_{min} * nbNotVisited$



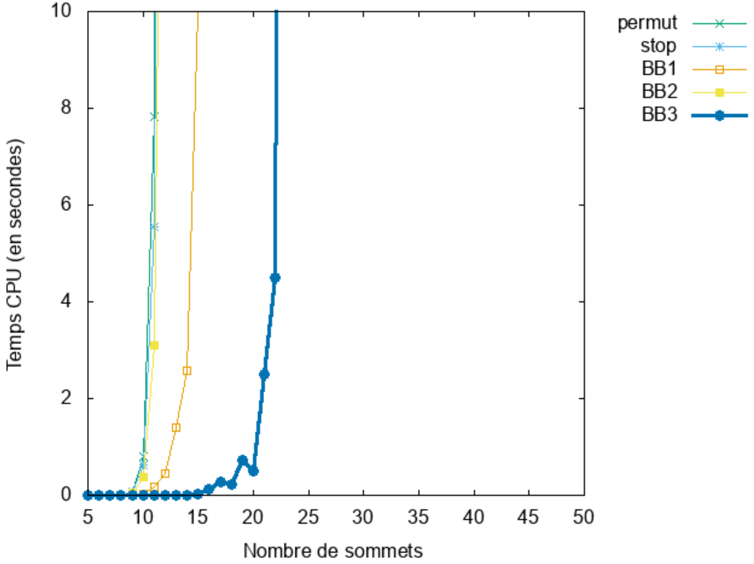
Results on Benchmark 2

Branch & Bound 2: Bound = $\sum_{i \in notVisited} \min_{j \in notVisited, j \neq i} d_{ij}$



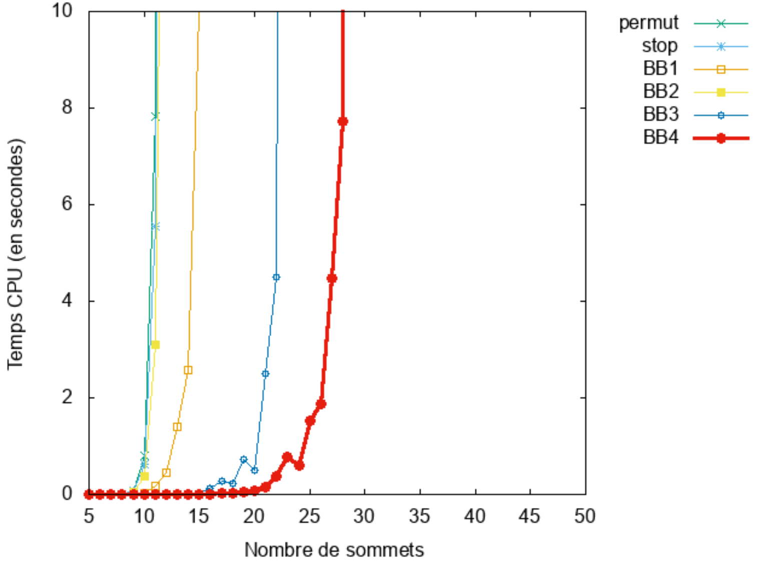
Results on Benchmark 2

Branch & Bound 3: Bound = minimal 1-tree cost



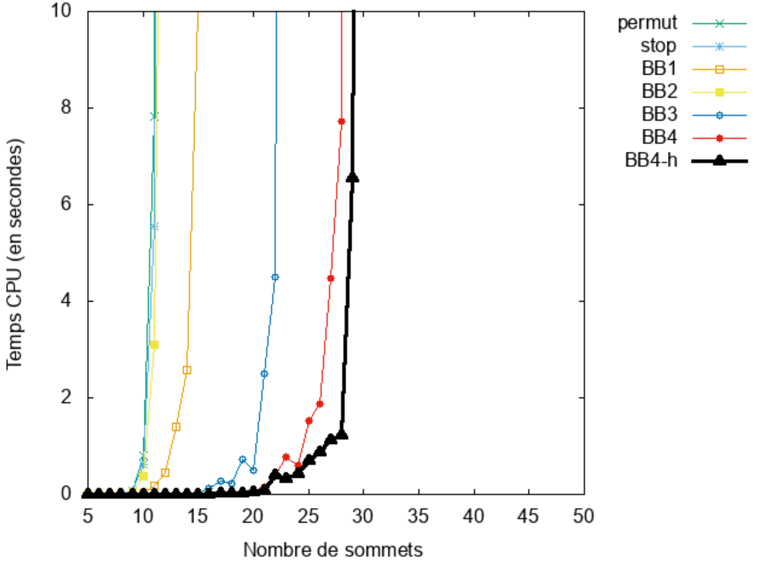
Results on Benchmark 2

Branch & Bound 4: Bound = subgradian opt. of Held-Karp (iterated 1-tree)



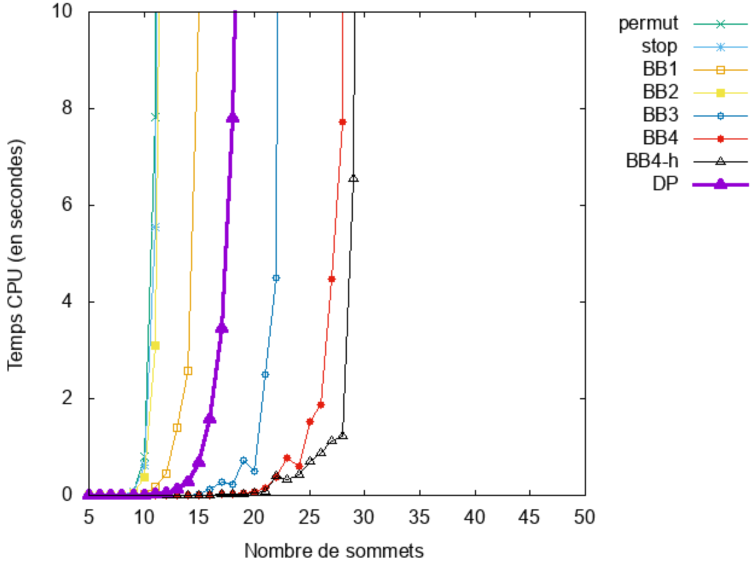
Results on Benchmark 2

Branch & Bound 4 + h: Addition of an ordering heuristic



Results on Benchmark 2

DPrec: Recursive Dynamic Programming $\rightsquigarrow \mathcal{O}(n^2 \cdot 2^n)$



Results on Benchmark 2

DPiter: Iterative Dynamic Programming $\rightsquigarrow \mathcal{O}(n^2 \cdot 2^n)$

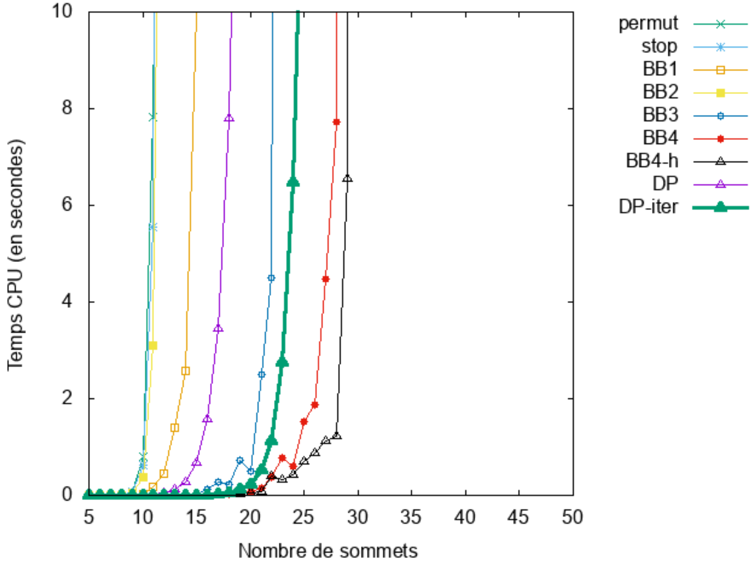
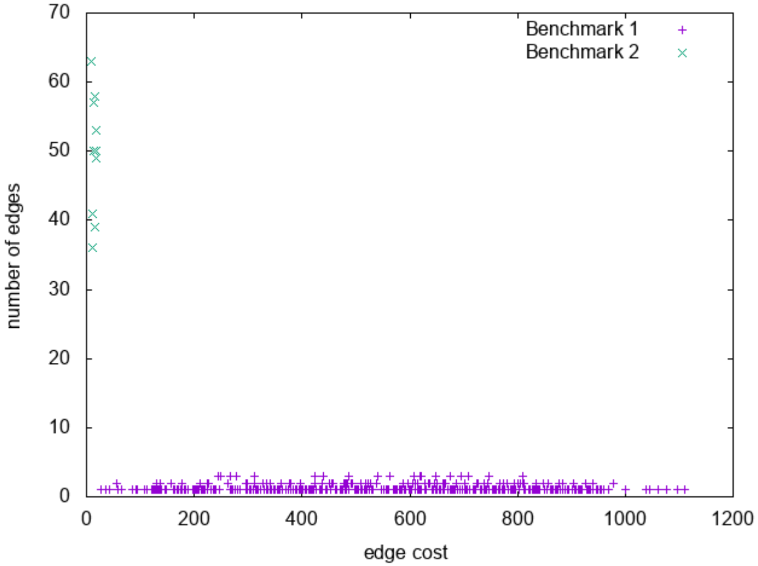


Illustration on the TSP

Comparison of Edge Cost Distributions on the 2 benchmarks



Plan

Code Tuning

Finer grain optimisation:

- Loops and procedures rather than algorithm paradigms
- Memory management rather than data structures

$\rightsquigarrow$ Small improvements... and loss of readability and generality!
$\rightsquigarrow$ Many of these optimisations are done by compilers (-O3 option of gcc)

We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil. D. Knuth

Example 1: Insertion Sort

```
for $i$ ranging from 1 to $n-1$ do
    /* Invariant: $tab[0..i-1]$ is sorted */
    $j \leftarrow i$
    while $j > 0$ and $tab[j] > tab[j-1]$ do
        exchange($tab[j], tab[j-1]$)
        $j \leftarrow j-1$
```

Possible optimisations?

	n=40000	n=80000	n=160000
Initial code	0.65	2.66	10.59

Example 1: Insertion Sort

```
for $i$ ranging from 1 to $n-1$ do
    /* Invariant: $tab[0..i-1]$ is sorted */
    $j \leftarrow i$; $x \leftarrow tab[i]$
    while $j > 0$ and $tab[j] > tab[j-1]$ do
        $tab[j] \leftarrow tab[j-1]$
        $j \leftarrow j-1$
    $tab[j] \leftarrow x$
```

Possible optimisations?

- Opt1: Memorise *tab*[*i*] before entering the loop

	n=40000		n=80000		n=160000	
Initial code	0.65		2.66		10.59	
Opt1	0.40	-38%	1.61	-40%	6.43	-39%

Example 1: Insertion Sort

```
$tab[0] \leftarrow -\infty$
for $i$ ranging from 1 to $n-1$ do
    /* Invariant: $tab[0..i-1]$ is sorted */
    $j \leftarrow i$; $x \leftarrow tab[i]$
    while ~~$j > 0$ and~~ $tab[j] > tab[j-1]$ do
        $tab[j] \leftarrow tab[j-1]$
        $j \leftarrow j-1$
    $tab[j] \leftarrow x$
```

Possible optimisations?

- Opt1: Memorise *tab*[*i*] before entering the loop
- Opt2: Add a sentinel value (assuming *tab*[0] is not used)

	n=40000		n=80000		n=160000	
Initial code	0.65		2.66		10.59	
Opt1	0.40	-38%	1.61	-40%	6.43	-39%
Opt2	0.67		2.72		10.91	

Example 1: Insertion Sort

```
$tab[0] \leftarrow -\infty$
for $i$ ranging from 1 to $n-1$ do
    /* Invariant: $tab[0..i-1]$ is sorted */
    $j \leftarrow i$; $x \leftarrow tab[i]$
    while $tab[j] > tab[j-1]$ do
        $tab[j] \leftarrow tab[j-1]$
        $j \leftarrow j-1$
    $tab[j] \leftarrow x$
```

Possible optimisations?

- Opt1: Memorise *tab*[*i*] before entering the loop
- Opt2: Add a sentinel value (assuming *tab*[0] is not used)

	n=40000		n=80000		n=160000	
Initial code	0.65		2.66		10.59	
Opt1	0.40	-38%	1.61	-40%	6.43	-39%
Opt2	0.67		2.72		10.91	
Opt1+Opt2	0.30	-54%	1.22	-54%	4.88	-54%

Example 2: Enumerate all permutations of an array

```
permut(int* tab, int k, int n)
begin
    if $k = n - 1$ then display(tab, n);
    else
        for i ranging from k to $n - 1$ do
            exchange(tab[k], tab[i])
            permut(tab, $k + 1$, n)
            exchange(tab[k], tab[i])
```

Possible optimisations?

n	Initial code	Opt1	Opt2	Opt1+Opt2
11	0.89			
13	143.64			

Example 2: Enumerate all permutations of an array

```
permut(int* tab, int k, int n)
begin
    if $k = n - 1$ then display(tab, n);
    else
        for i ranging from k to $n - 1$ do
            exchange(tab[k], tab[i])
            permut(tab, $k + 1$, n)
            exchange(tab[k], tab[i])
```

Possible optimisations?

- Opt1: Unfold *exchange* (inlining procedure call)

n	Initial code	Opt1	Opt2	Opt1+Opt2
11	0.89	0.63		
13	143.64	97.60		

Example 2: Enumerate all permutations of an array

```
permut(int* $tab$, int $k$, int $n$)
begin
    if $k = n - 1$ then display($tab, n$);
    else
        for $i$ ranging from $k$ to $n - 1$ do
            exchange($tab[k], tab[i]$)
            permut($tab, k + 1, n$)
            exchange($tab[k], tab[i]$)
```

```
if $k = n - 1$ then display($tab, n$);
else
    for $i$ ranging from $k$ to $n - 1$ do
        exchange($tab[k], tab[i]$)
        for $j$ from $k + 1$ to $n - 1$ do
            exchange($tab[k + 1], tab[i]$)
            permut2($tab, k + 2, n$)
            exchange($tab[k + 1], tab[i]$)
        exchange($tab[k], tab[i]$)
```

Possible optimisations?

- Opt1: Unfold *exchange* (inlining procedure call)
- Opt2: Divide by 2 the number of recursive calls (Assumption: n odd)

n	Initial code	Opt1	Opt2	Opt1+Opt2
11	0.89	0.63	0.82	
13	143.64	97.60	126.21	

Example 2: Enumerate all permutations of an array

```
permut(int* tab, int k, int n)
begin
    if $k = n - 1$ then display(tab, n);
    else
        for i ranging from k to $n - 1$ do
            exchange(tab[k], tab[i])
            permut(tab, $k + 1$, n)
            exchange(tab[k], tab[i])
```

```
if $k = n - 1$ then display(tab, n);
else
    for i ranging from k to $n - 1$ do
        exchange(tab[k], tab[i])
        for j from $k + 1$ to $n - 1$ do
            exchange(tab[$k + 1$], tab[i])
            permut2(tab, $k + 2$, n)
            exchange(tab[$k + 1$], tab[i])
        exchange(tab[k], tab[i])
```

Possible optimisations?

- Opt1: Unfold *exchange* (inlining procedure call)
- Opt2: Divide by 2 the number of recursive calls (Assumption: *n* odd)

n	Initial code	Opt1	Opt2	Opt1+Opt2
11	0.89	0.63	0.82	0.56
13	143.64	97.60	126.21	85.20

Example 2: Enumerate all permutations of an array

```
permut(int* tab, int k, int n)
begin
    if $k = n - 1$ then display(tab, n);
    else
        for i ranging from k to $n - 1$ do
            exchange(tab[k], tab[i])
            permut(tab, $k + 1$, n)
            exchange(tab[k], tab[i])
```

```
if $k = n - 1$ then display(tab, n);
else
    for i ranging from k to $n - 1$ do
        exchange(tab[k], tab[i])
        for j from $k + 1$ to $n - 1$ do
            exchange(tab[$k + 1$], tab[i])
            permut2(tab, $k + 2$, n)
            exchange(tab[$k + 1$], tab[i])
        exchange(tab[k], tab[i])
```

Possible optimisations?

- Opt1: Unfold *exchange* (inlining procedure call)
- Opt2: Divide by 2 the number of recursive calls (Assumption: *n* odd)

n	Initial code		Opt1		Opt2		Opt1+Opt2	
11	0.89	0.35	0.63	0.34	0.82	0.28	0.56	0.28
13	143.64	52.92	97.60	52.87	126.21	44.28	85.20	44.27

Results with the -O3 option of gcc

$\rightsquigarrow$ In many cases, we'd better let the compiler do optimisations!

Tools for Algorithm and Code Tuning

Profilers:

- gprof (gcc)
- Cachegrind and Callgrind (Valgrind)
- Instruments (Xcode)
- ...

Time spent in each function (percentage and absolute value)
$\leadsto$ Not always compatible with compiler optimisations!

Tools for the experimental evaluation and data analysis

Experimentally check that your optimisations actually optimise the program!

Illustration 1: Optimisation of *AntClique*

MaxClique Problem (recall)

- Input: a graph $G = (V, E)$
- Output: Largest subset $C \subseteq V$ such that $\forall \{i, j\} \subseteq C, \{i, j\} \in E$

***AntClique*:**

- Incomplete algorithm: May find a sub-optimal solution
- Based on the Ant Colony Optimization (ACO) meta-heuristic
  $\leadsto$ Particular kind of reinforcement learning

Reference:

C. Solnon & S. Fenet: *A study of ACO capabilities for solving the Maximum Clique Problem*, Journal of Heuristics, 12(3):155-180, Springer, 2006

Basic Idea of AntClique

- initialize pheromone trails
- repeat
  1. each ant builds a clique
  2. update pheromone trails
- until optimal clique found or stagnation

Basic Idea of AntClique

- **initialize pheromone trails**
- repeat
  1. each ant builds a clique
  2. update pheromone trails
- until optimal clique found or stagnation

Pheromone is laid on edges:

$\rightsquigarrow \tau(i,j) =$ learned desirability of selecting both *i* and *j* in a same clique

Initialize $\tau(i,j)$ to τ_{max}, for each edge $\{i,j\} \in E$

$\rightsquigarrow \tau_{max}$ = parameter

Basic Idea of AntClique

```
• initialize pheromone trails
• repeat
    1 each ant builds a clique
    2 update pheromone trails
• until optimal clique found or stagnation
```

Greedy randomized construction of a clique $\mathcal{C}$

- Randomly choose $i \in V$ and initialize $\mathcal{C}$ to $\{i\}$
- While $cand = \{j \in V \setminus \mathcal{C} : \forall i \in \mathcal{C}, \{i,j\} \in E\} \neq \emptyset$:
  - Select randomly a vertex $v_j \in cand$ wrt probability
    $$p(v_j) = \frac{[\sum_{i \in \mathcal{C}} \tau(i,j)]^\alpha}{\sum_{k \in cand} [\sum_{i \in \mathcal{C}} \tau(i,k)]^\alpha}$$
    where α = pheromone weight (parameter)
  - Add v_j to $\mathcal{C}$
- Return $\mathcal{C}$

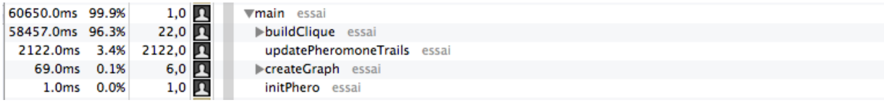
Basic Idea of AntClique

- initialize pheromone trails
- repeat
  1. each ant builds a clique
  2. **update pheromone trails**
- until optimal clique found or stagnation

Pheromone updating step

- Evaporation: multiply pheromone trails by $(1 - \rho)$
  $\rightsquigarrow \rho$ = evaporation rate $(0 \leq \rho \leq 1)$
- Reward: add pheromone on all edges of the best clique
- Bound all pheromone trails to prevent early stagnation:
  - If $\tau(i,j) < \tau_{min}$ then $\tau(i,j) \leftarrow \tau_{min}$
  - If $\tau(i,j) > \tau_{max}$ then $\tau(i,j) \leftarrow \tau_{max}$

- Profiling of `main`

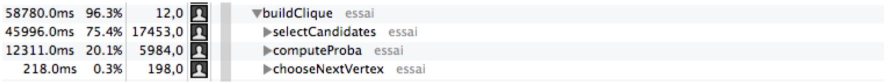


```
60650.0ms  99.9%     1,0   ▼main  essai
58457.0ms  96.3%    22,0    ▶buildClique  essai
 2122.0ms   3.4%  2122,0     updatePheromoneTrails  essai
   69.0ms   0.1%     6,0    ▶createGraph  essai
    1.0ms   0.0%     1,0     initPhero  essai
```

- 96.3% of the time spent in `buildClique`
  $\rightsquigarrow$ Zoom on `buildClique`

```
clique[0] = getNextRand(G->nbVertices);
cliqueSize = 1;
nbCandidates = selectCandidates(cliqueSize, clique, candidates, G);
while (nbCandidates>0){
    computeProba(nbCandidates, candidates, cliqueSize, clique, alpha, G, p);
    clique[cliqueSize++] = candidates[chooseNextVertex(p, nbCandidates)];
    nbCandidates = selectCandidates(cliqueSize, clique, candidates, G);
}
```

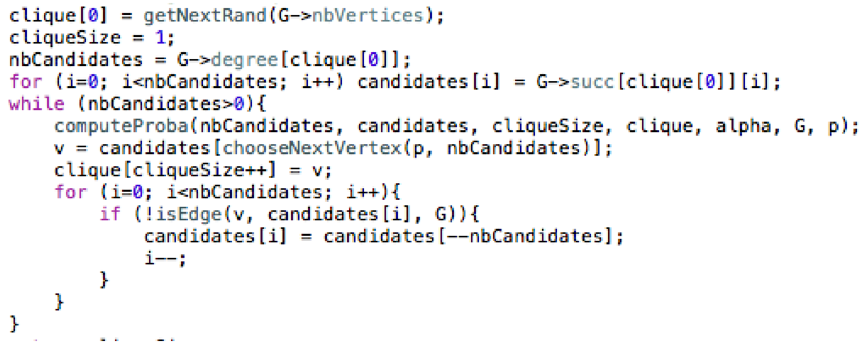
- Profiling of `buildClique`



```
58780.0ms  96.3%     12,0   ▼buildClique  essai
45996.0ms  75.4%  17453,0    ▶selectCandidates  essai
12311.0ms  20.1%   5984,0    ▶computeProba  essai
  218.0ms   0.3%    198,0    ▶chooseNextVertex  essai
```

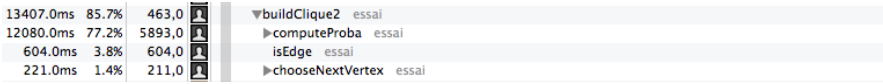
- 75.4% of the time spent in `selectCandidates`
  $\rightsquigarrow$ Opt1: Incrementally maintain the candidate list

- Code of `buildClique2`:



```
clique[0] = getNextRand(G->nbVertices);
cliqueSize = 1;
nbCandidates = G->degree[clique[0]];
for (i=0; i<nbCandidates; i++) candidates[i] = G->succ[clique[0]][i];
while (nbCandidates>0){
    computeProba(nbCandidates, candidates, cliqueSize, clique, alpha, G, p);
    v = candidates[chooseNextVertex(p, nbCandidates)];
    clique[cliqueSize++] = v;
    for (i=0; i<nbCandidates; i++){
        if (!isEdge(v, candidates[i], G)){
            candidates[i] = candidates[--nbCandidates];
            i--;
        }
    }
}
```

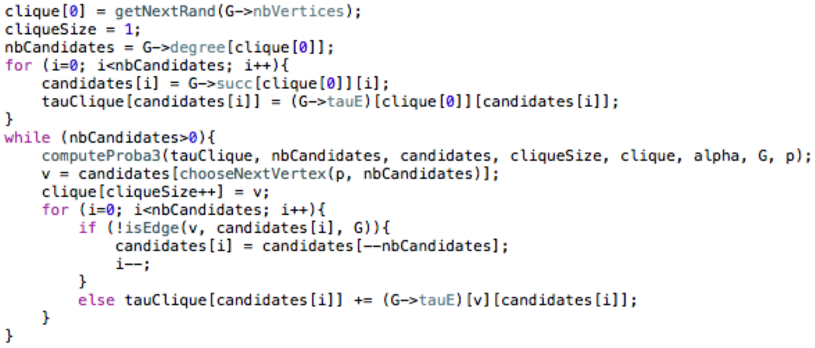
- Profiling of `buildClique2`



```
13407.0ms  85.7%   463,0   ▼buildClique2  essai
12080.0ms  77.2%  5893,0    ▶computeProba  essai
  604.0ms   3.8%   604,0     isEdge  essai
  221.0ms   1.4%   211,0    ▶chooseNextVertex  essai
```

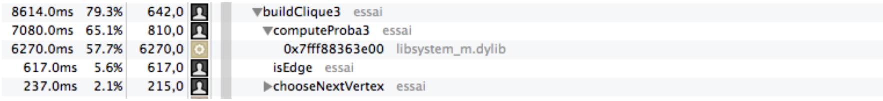
- 77.2% of the time spent in `computeProba`
  $\rightsquigarrow$ Opt2: Incrementally maintain the pheromone factor

- Code of `buildClique3`:



```
clique[0] = getNextRand(G->nbVertices);
cliqueSize = 1;
nbCandidates = G->degree[clique[0]];
for (i=0; i<nbCandidates; i++){
    candidates[i] = G->succ[clique[0]][i];
    tauClique[candidates[i]] = (G->tauE)[clique[0]][candidates[i]];
}
while (nbCandidates>0){
    computeProba3(tauClique, nbCandidates, candidates, cliqueSize, clique, alpha, G, p);
    v = candidates[chooseNextVertex(p, nbCandidates)];
    clique[cliqueSize++] = v;
    for (i=0; i<nbCandidates; i++){
        if (!isEdge(v, candidates[i], G)){
            candidates[i] = candidates[--nbCandidates];
            i--;
        }
        else tauClique[candidates[i]] += (G->tauE)[v][candidates[i]];
    }
}
```

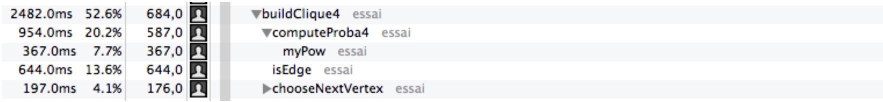
- Profiling of `buildClique3`



```
8614.0ms  79.3%   642,0   ▼buildClique3  essai
7080.0ms  65.1%   810,0    ▼computeProba3  essai
6270.0ms  57.7%  6270,0       0x7fff88363e00  libsystem_m.dylib
 617.0ms   5.6%   617,0     isEdge  essai
 237.0ms   2.1%   215,0    ▶chooseNextVertex  essai
```

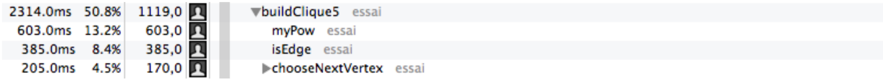
- 57.7% of the time spent in `pow` (from `math.h`)
  $\rightsquigarrow$ Opt3: replace `pow` with `myPow` !

- Profiling of `buildClique4`



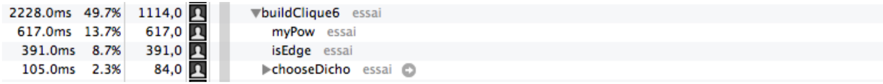
```
2482.0ms  52.6%   684,0   ▼buildClique4  essai
 954.0ms  20.2%   587,0    ▼computeProba4  essai
 367.0ms   7.7%   367,0       myPow  essai
 644.0ms  13.6%   644,0     isEdge  essai
 197.0ms   4.1%   176,0    ▶chooseNextVertex  essai
```

- 20.2% of the time spent in `computeProba4`
  ⇝ Opt4: merge the loop that computes proba. with candidate filtering
- Profiling of `buildClique5`



```
2314.0ms  50.8%  1119,0   ▼buildClique5  essai
 603.0ms  13.2%   603,0     myPow  essai
 385.0ms   8.4%   385,0     isEdge  essai
 205.0ms   4.5%   170,0    ▶chooseNextVertex  essai
```

- A last optimisation?
  ⇝ Opt5: replace the sequential search of `chooseNextVertex` with a dichotomous search
- Profiling of `buildClique6`



```
2228.0ms  49.7%  1114,0   ▼buildClique6  essai
 617.0ms  13.7%   617,0     myPow  essai
 391.0ms   8.7%   391,0     isEdge  essai
 105.0ms   2.3%    84,0    ▶chooseDicho  essai
```

Gains are getting smaller and smaller . . . Is it still useful?

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	
C125.9	3.61	
C250.9	8.34	
C500.9	23.53	
C1000.9	111.30	
C2000.9	347.15	

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	
C125.9	3.61	1.79	
C250.9	8.34	3.65	
C500.9	23.53	8.49	
C1000.9	111.30	28.94	
C2000.9	347.15	88.18	

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	Opt2	
C125.9	3.61	1.79	1.29	
C250.9	8.34	3.65	2.78	
C500.9	23.53	8.49	5.84	
C1000.9	111.30	28.94	13.52	
C2000.9	347.15	88.18	27.32	

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	Opt2	Opt3	
C125.9	3.61	1.79	1.29	0.32	
C250.9	8.34	3.65	2.78	0.71	
C500.9	23.53	8.49	5.84	1.59	
C1000.9	111.30	28.94	13.52	4.06	
C2000.9	347.15	88.18	27.32	10.64	

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	Opt2	Opt3	Opt4	
C125.9	3.61	1.79	1.29	0.32	0.24	
C250.9	8.34	3.65	2.78	0.71	0.51	
C500.9	23.53	8.49	5.84	1.59	1.21	
C1000.9	111.30	28.94	13.52	4.06	3.32	
C2000.9	347.15	88.18	27.32	10.64	9.14	

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	Opt2	Opt3	Opt4	Opt5	$\frac{\text{init}}{\text{Opt5}}$
C125.9	3.61	1.79	1.29	0.32	0.24	0.24	15
C250.9	8.34	3.65	2.78	0.71	0.51	0.51	16
C500.9	23.53	8.49	5.84	1.59	1.21	1.11	21
C1000.9	111.30	28.94	13.52	4.06	3.32	2.98	37
C2000.9	347.15	88.18	27.32	10.64	9.14	8.81	39

Experimental Comparison (with -O3!)

- Initial code
- Opt1: Incrementally maintain candidates
- Opt2: Incrementally maintain pheromone factor
- Opt3: Replace `pow` of `math.h` with an *ad-hoc* function
- Opt4: Merge loops
- Opt5: Dichotomous search of the selected vertex

	Init	Opt1	Opt2	Opt3	Opt4	Opt5	$\frac{\text{init}}{\text{Opt5}}$
C125.9	3.61	1.79	1.29	0.32	0.24	0.24	15
C250.9	8.34	3.65	2.78	0.71	0.51	0.51	16
C500.9	23.53	8.49	5.84	1.59	1.21	1.11	21
C1000.9	111.30	28.94	13.52	4.06	3.32	2.98	37
C2000.9	347.15	88.18	27.32	10.64	9.14	8.81	39
C2000.5	33.64	11.37	6.23	4.32	4.15	4.03	8
C4000.5	85.53	30.50	18.73	14.75	14.17	14.02	6

Scale-up Properties of the 6 Variants

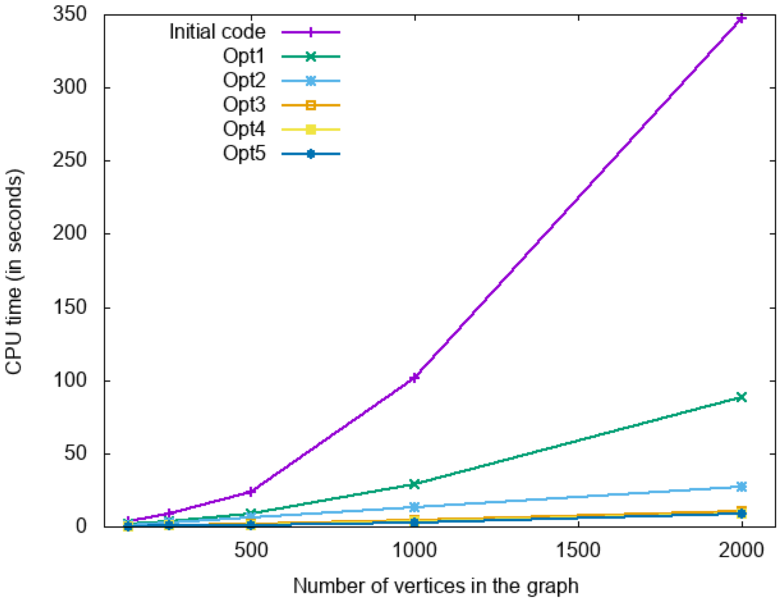


Illustration 2: LAD

Subgraph Isomorphism Problem (recall):

Given $G_p = (V_p, E_p)$ and $G_t = (V_t, E_t)$, find an injective function $f : V_p \rightarrow V_t$ such that $\forall (u, v) \in E_p, (f(u), f(v)) \in E_t$

Exact constraint-based approach LAD[1]:

$\forall u \in V_p$, maintain the set $D(u)$ of target vertices that may be matched with u

- $\forall v \in D(u)$, every neighbour of u must be matched with a different vertex in the neighbourhood of v
- Every pattern vertex must be matched with a different target vertex

$\rightsquigarrow$ Extended to PathLAD[2] by exploiting invariant properties[3]

References:

(1) Solnon: *Alldifferent-based filtering for subgraph isomorphism*, in AI 2010

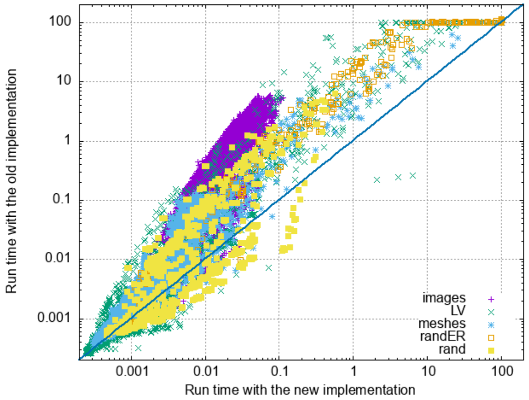
(2) Kotthoff, McCreesh, Solnon: *Portfolios of Subgraph Isomorphism Algorithms*, in Learning and Intelligent OptimizatioN Conference (LION), 2016

(3) McCreesh, Prosser: *A parallel, backjumping subgraph isomorphism algorithm using supplemental graphs*, in CP 2015

Refactoring of LAD

Improve performance without changing the number of explored nodes:

- Tarjan instead of Kosaraju for searching for SCC
- Ford-Fulkerson instead of Hopcroft-Karp for augmenting paths
- Data structures: Sparse sets, timestamps, ...



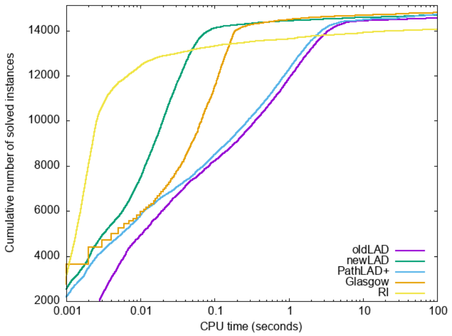
Speed-up:

- images : 38.9
- LV : 7.6
- meshes : 3.8
- randER : 11.9
- rand : 6.5

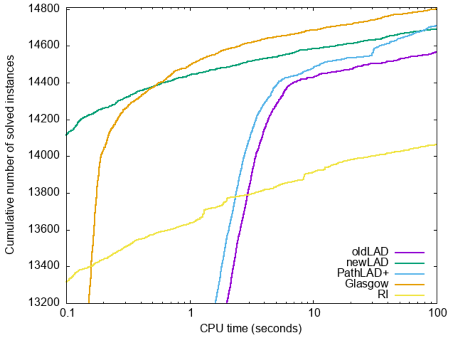
Is it enough to outperform the state-of-the-art?

Comparison with state-of-the-art approaches

Big picture:



With a zoom:



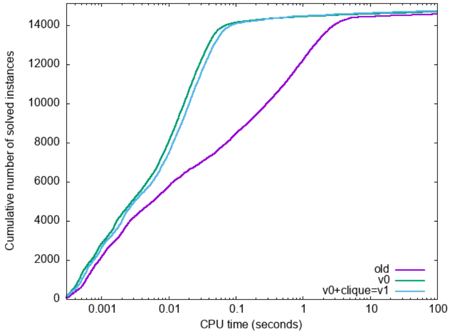
newLAD is outperformed by:

- RI for short time limits (<0.04s)
- Glasgow for long time limits (>0.5s)

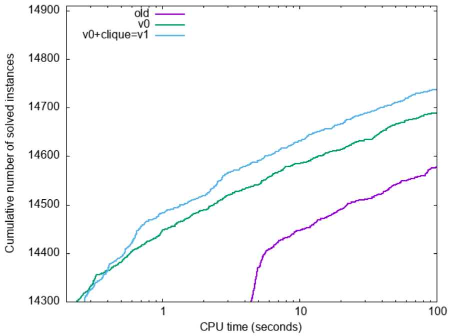
$\leadsto$ We need to improve the algorithm, not just the code!

Improvement of LAD algorithm

Big picture:



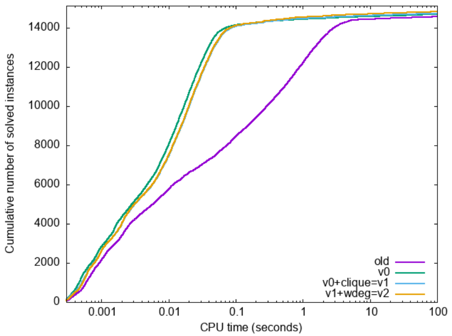
With a zoom:



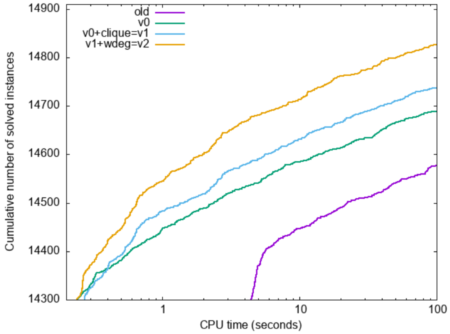
- New invariant properties (cliques of order 4, 5, and 6)
- New variable ordering heuristic (wdeg)
- Random restarts + nogood learning
- New value ordering heuristic
- Replace LAD filtering with a cheaper one when density > 15%

Improvement of LAD algorithm

Big picture:



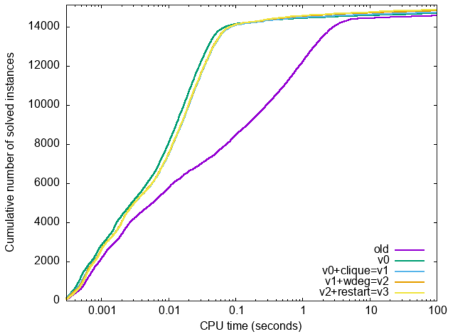
With a zoom:



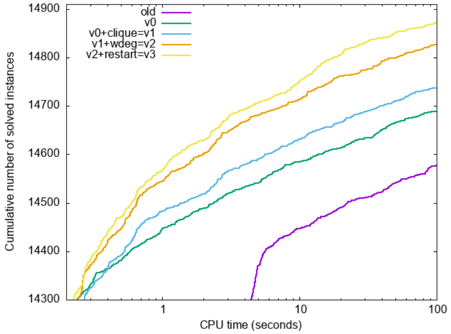
- New invariant properties (cliques of order 4, 5, and 6)
- New variable ordering heuristic (wdeg)
- Random restarts + nogood learning
- New value ordering heuristic
- Replace LAD filtering with a cheaper one when density > 15%

Improvement of LAD algorithm

Big picture:



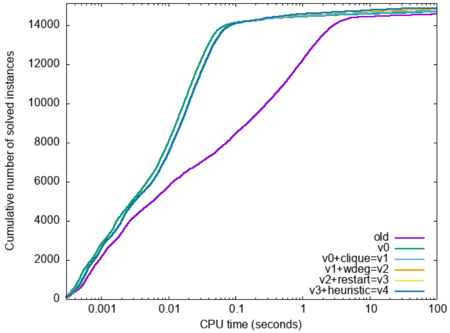
With a zoom:



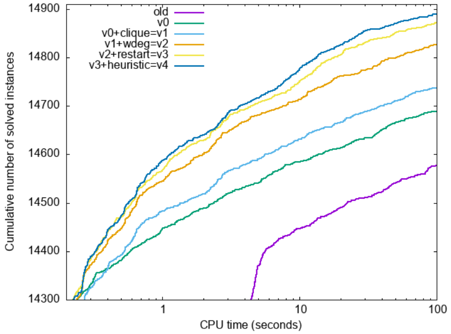
- New invariant properties (cliques of order 4, 5, and 6)
- New variable ordering heuristic (wdeg)
- Random restarts + nogood learning
- New value ordering heuristic
- Replace LAD filtering with a cheaper one when density > 15%

Improvement of LAD algorithm

Big picture:



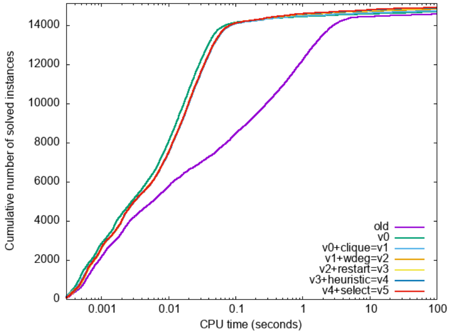
With a zoom:



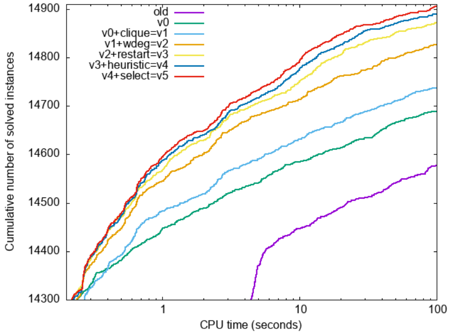
- New invariant properties (cliques of order 4, 5, and 6)
- New variable ordering heuristic (wdeg)
- Random restarts + nogood learning
- New value ordering heuristic
- Replace LAD filtering with a cheaper one when density > 15%

Improvement of LAD algorithm

Big picture:



With a zoom:



- New invariant properties (cliques of order 4, 5, and 6)
- New variable ordering heuristic (wdeg)
- Random restarts + nogood learning
- New value ordering heuristic
- Replace LAD filtering with a cheaper one when density > 15%

Plan

Parameters and Hyper-Parameters

Parameters = Variables that define thresholds, weights, frequencies, . . .

- Parameters change the algorithm performance
- Examples:
    - Simulated Annealing: Initial temperature, Cooling rate
    - Tabu Search: Tabu list length
    - GA: Population size, Cross-over rate, Mutation rate

Hyper-parameters = Variables that correspond to design choices

- Hyper-parameters change the algorithm
- Examples:
    - Branch & Bound: Bound function
    - Local Search: Neighborhood function
    - Constraint Programming: Filtering algorithm

Both param. and hyper-param. are called "Parameters" in what follows

The Vocabulary of Experimentation (recalls)

Factors = Parameters that are studied in the experiment

$\rightsquigarrow$ Identify "important" parameters, and fix the other parameters

Levels = Set of possible values for a factor

- Symbolic factor: 1 level per value
- Numeric factor: Identify intervals of relevant values by sampling
  $\rightsquigarrow$ Use a geometric serie to sample: 1, 2, 4, 8, . . . or 1, 10, 100, . . .

Configuration = An assignment of one level to each factor

Design Point = Configuration that must be experimentally evaluated

- Full factorial design = All Factor/Level combinations (grid search)
  - Pros: Identify all factor effects, including interaction effects due to inter-dependency of factors
  - Cons: Exponential number of combinations wrt number of factors
- Fractional factorial design = Selection of a subset of configurations
  $\rightsquigarrow$ **How to select configurations that must be evaluated?**

Manual Tuning vs Automatic Configuration

Main drawbacks of manual parameter tuning:

- It is time consuming
- Intuitions may be misleading
- It may be unfair
  $\leadsto$ Are we spending the same time for tuning all approaches?
- The tuning step is not reproducible

Programming by Optimisation [Hoos 2012]:

Developers specify a potentially large design space of programs that accomplish a given task, from which versions of the program optimised for various use contexts are generated automatically.

Automatic Configuration

Definition of the problem:

Given:

- A set of configurations Θ of an algorithm A
- A distribution $\mathcal{D}$ over the set of instances $\mathcal{I}$ of the problem solved by A
- A performance measure $m : \Theta \times \mathcal{I} \to \mathbb{R}$

Search for $\theta^* \in \Theta$ which optimises the expectation of $m(\theta^*, i)$ when $i \sim \mathcal{D}$

How to define the distribution $\mathcal{D}$?

- $\mathcal{D}$ should be representative of the actual instances that must be solved
  $\rightsquigarrow$ Gather a set $\mathcal{S}$ of representative instances

How to obtain training instances from $\mathcal{S}$?

- Solution 1: Design a model for randomly generating instances that have the same distribution as $\mathcal{S}$
- Solution 2: Use $\mathcal{S}$ as a finite support definition of $\mathcal{D}$
  $\rightsquigarrow$ Split $\mathcal{S}$ into training and test sets for cross-validation

Example of Automatic Configuration Tool

$\rightsquigarrow$ **Sequential Model-based Algorithm Configuration (SMAC)**

Basic Idea:

- Perform an initial set $\mathcal{R}$ of runs and select a first configuration θ^*
- Iterate the following steps:
  - Use $\mathcal{R}$ to build a model for predicting configuration performances
  - Use that model to select promising configurations
  - For each selected configuration θ:
    - Compare θ with θ^* using Random Online Agressive Racing (ROAR)
    - Update θ^* if θ wins the race, and update the set $\mathcal{R}$ of runs

Reference:

F. Hutter, H. Hoos, K. Leyton-Brown (2011): *Sequential Model-Based Optimization for General Algorithm Configuration*. LION

Source code available at

`http://www.cs.ubc.ca/labs/beta/Projects/SMAC/`

Some other Automatic Configuration Tools

ParamILS: Greedy Local Search with Restarts

F. Hutter, H. Hoos, K. Leyton-Brown, T. Stützle (2009): *ParamILS: An Automatic Algorithm Configuration Framework*. JAIR

Source code available at
`http://www.cs.ubc.ca/labs/beta/Projects/ParamILS/`

Iterated F-race: Iteratively sample configurations to race

M. Lopez-Ibanez, J. Dubois-Lacoste, L. Perez Caceres, M. Birattari, T. Stützle (2016): *The irace package: Iterated racing for automatic algorithm configuration*. Operations Research Perspectives

Available as a R package

Plan

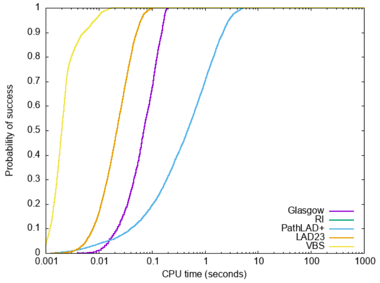
From Configuration to Selection

Automatic configuration finds the Single Best Solver (SBS)...

...But SBS may be far from VBS when instances are heterogeneous

Illustration on the subgraph isomorphism problem

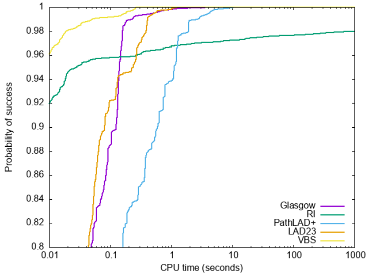
CDF for Image instances:



- SBS = VBS = RI

$\leadsto$ No need for per-instance selection

CDF for Rand instances:



- SBS depends on time limit
- VBS outperforms SBSs

$\leadsto$ Use per-instance selection!

Per Instance Algorithm Selection

Definition of the problem:

Given a portfolio $\mathcal{P}$ of algorithms (or of algorithm configurations) and an instance i, select an algorithm $A \in \mathcal{P}$ expected to perform best on i

Offline training:

Given:

- A distribution $\mathcal{D}$ over the set of instances $\mathcal{I}$
- A performance measure $m : \mathcal{P} \times \mathcal{I} \to \mathbb{R}$
- An embedding function $f : \mathcal{I} \to \mathcal{F}$ where $\mathcal{F} \subseteq \mathbb{R}^m$ is the feature space
  $\leadsto$ Each instance $i \in \mathcal{I}$ is described by $f(i) \in \mathcal{F}$

Build a selector $S : \mathcal{F} \to \mathcal{P}$ which optimises $m(S(f(i)), i)$ when $i \sim \mathcal{D}$

Online selection of an algorithm for an instance $i \in \mathcal{I}$

Return $S(f(i))$

Examples of existing Automatic Selection Approaches

SATzilla:

- Offline: Learn a model for each algorithm
  $\leadsto$ Prediction of performance given instance features
- Online selection of an algorithm to solve a new instance *i*:
  $\leadsto$ Predict performance for each algorithm
  $\leadsto$ Select the algorithm with the best predicted performance

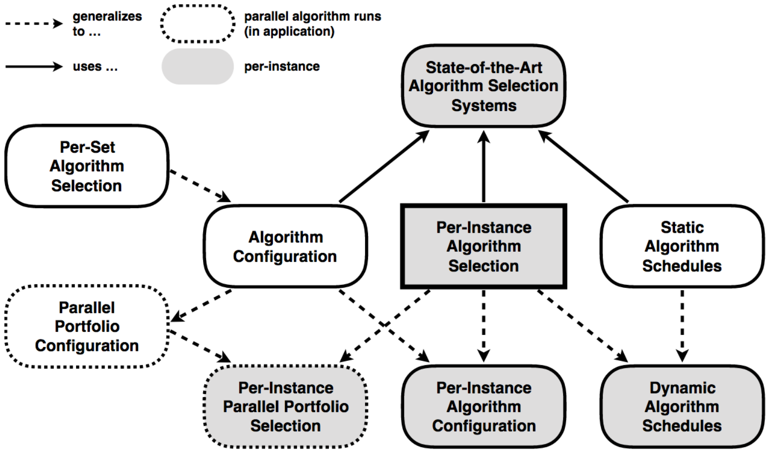
See L. Xu, F. Hutter, H. H. Hoos, K. Leyton-Brown (2009): SATzilla2009: an Automatic Algorithm Portfolio for SAT . SAT Competition 2009

ISAC:

- Offline: Partition instances into homogeneous clusters and use automatic configuration to determine the best algorithm for each cluster
- Online selection of an algorithm to solve a new instance *i*:
  $\leadsto$ Search for the cluster of *i* and select the corresponding algorithm

See Y. Malitsky: Instance-Specific Algorithm Configuration, PhD thesis, Brown University, 2012

Related Problems

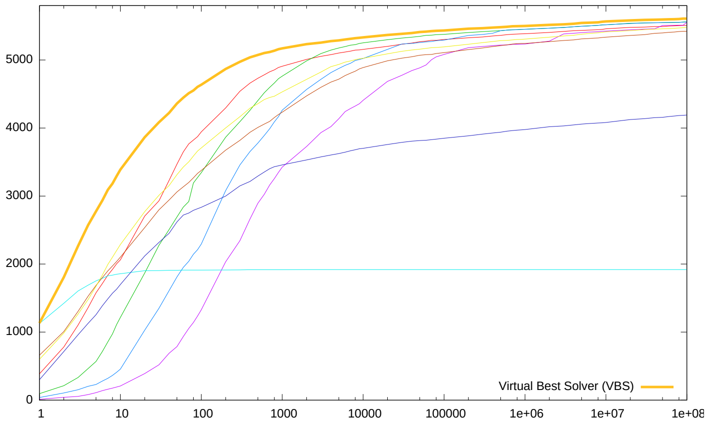

generalizes to ...
uses ...
parallel algorithm runs (in application)
per-instance
State-of-the-Art Algorithm Selection Systems
Per-Set Algorithm Selection
Algorithm Configuration
Per-Instance Algorithm Selection
Static Algorithm Schedules
Parallel Portfolio Configuration
Per-Instance Parallel Portfolio Selection
Per-Instance Algorithm Configuration
Dynamic Algorithm Schedules

Reference:

P. Kerschke, H. Hoos, F. Neumann, H. Trautmann (2019): *Automated Algorithm Selection: Survey and Perspectives.* ECJ

Illustration: Algorithm Selection for Subgraph Isomorphism

$\rightsquigarrow$ **CDF of 8 algorithms + VBS**



Reference:

L. Kotthoff, C. McCreesh, C. Solnon: *Portfolios of Subgraph Isomorphism Algorithms*, in 10th International Conference on Learning and Intelligent OptimizatioN Conference (LION), 2016

Overview of the process

Offline:

- Describe each training instance by a feature vector
- Train a model that predicts the best algorithm for each training instance

Online: Solve a new instance $i \in \mathcal{I}$

- Sequentially run 2 very fast and complementary algorithms
  $\rightsquigarrow$ Solve very easy instances
  $\rightsquigarrow$ Collect dynamic features for instances that are not solved
- If instance not solved:
  - Extract features from i
  - Ask the model to select an algorithm given the features
  - Run the algorithm

Feature extraction

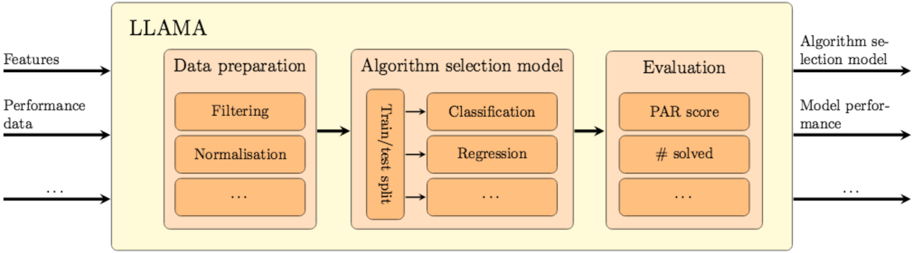
Static features extracted from the graphs

- Number of vertices and edges
- Density
- Number of loops
- Mean and max. degrees
- Mean and max. distance between all pairs of vertices
- Proportion of vertex pairs which are at least 2, 3 and 4 apart
- Binary features: Regular? Connected?

Dynamic features collected when running the 2 algorithms

- Number of value removals
- Percentage (average, min and max) of removed values per variable
- Algorithm solving time

Selection model: LLAMA



- R package for designing algorithm selectors
  https://bitbucket.org/lkotthoff/llama
- Includes different models
  $\rightsquigarrow$ Best results: Pairwise regression approach with random forest regression
  - For each pair of algorithm, train a model to predict performance difference
  - Choose algorithm with highest cumulative performance difference

Experimental evaluation (1/2)

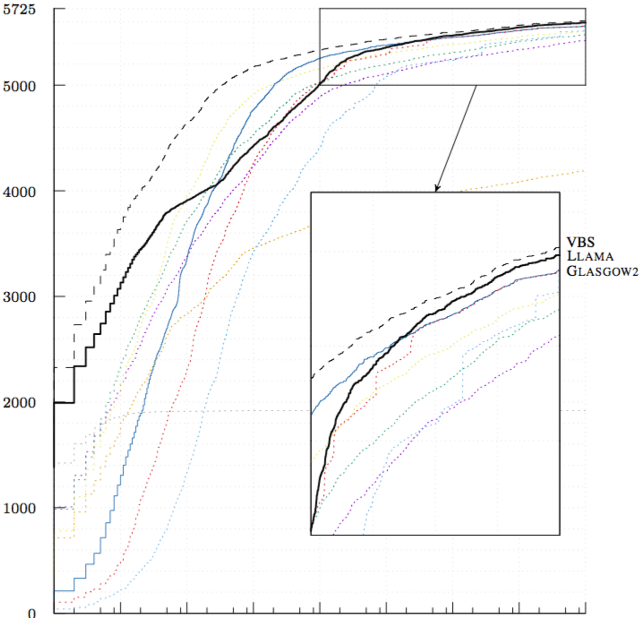
Experimental setup:

- 10-fold cross-validation
- Performance measures:
  - MCP: MisClassification Penalty
    $\rightsquigarrow$ Additional time required to solve an instance wrt VBS
  - # solved = number of instances that are solved
  - Time: time required to solve the instance, or 10^8 if not solved
    $\rightsquigarrow$ Lower bound of the actual time

Results:

Model	Mean MCP	# solved	Mean time
VBS	0	$5,608$	$2,375,913$
LLAMA	$287,704$	$5,592$	$2,664,293$
SBS	$798,660$	$5,562$	$3,174,573$

Experimental evaluation (2/2)



Plan du cours

Take away message?

Computer science is a science...

... where theory and practice should be combined!

- Theoretical analysis of algorithms
  - Study problem complexities before designing algorithms
  - Study the theoretical complexity of your algorithms
  - Prove properties of algorithms and codes
- Experimental analysis of algorithms
  - Choose benchmarks, factors, design points, and performance measures
  - Analyse results
  - Make it reproducible
- Algorithm engineering
  - Algorithm tuning vs code tuning
    $\leadsto$ Find the right compromise between efficiency and readability
  - Parameter tuning
    $\leadsto$ Use tools to automate parameter setting

Final words by Don Knuth

Computer programming is an art, because it applies accumulated knowledge to the world, because it requires skill and ingenuity, and especially because it produces objects of beauty. A programmer who subconsciously views himself as an artist will enjoy what he does and will do it better.

We should continually be striving to transform every art into a science: in the process, we advance the art.

An algorithm must be seen to be believed.