Hybrid metaheuristics for the *Far From Most String Problem*

Daniele Ferone[1], Paola Festa[1], and Mauricio G.C. Resende[2]

[1]Department of Mathematics and Applications "R. Caccioppoli"
University of Napoli FEDERICO II, Italy
E-mails: paola.festa@unina.it, danieleferone@gmail.com

[2]AT&T Labs Research, Florham Park, NJ, USA
Email: mgcr@research.att.com

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- given two sequences s^i and s^l on Σ such that $|s^i| = |s^l|$, $d_H(s^i, s^l)$ denotes their Hamming distance and is given by

$$d_H(s^i, s^l) = \sum_{j=1}^{|s^i|} \Phi(s^i_j, s^l_j), \qquad (1)$$

where s^i_j and s^l_j are the characters in position j in s^i and s^l, respectively, and $\Phi : \Sigma \times \Sigma \to \{0, 1\}$ is the predicate function such that

$$\Phi(a, b) = \begin{cases} 0, & \text{if } a = b; \\ 1, & \text{otherwise.} \end{cases}$$

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$$\Phi(a, b) = \begin{cases} 0, & \text{if } a = b; \\ 1, & \text{otherwise.} \end{cases}$$

- a set of sequences $\Omega = \{s^1, s^2, \ldots, s^n\}$ on Σ ($s^i \in \Sigma^m$, $i = 1, \ldots, n$)

Definition (Far From Most String Problem)

The FFMSP consists in determining a sequence far from as many as possible sequences in the input set Ω. This can be formalized by saying that given a threshold t, a string s must be found maximizing the variable x such that

$$d_H(s, \bar{s}) \geq t, \mathit{for}\ \bar{s} \in P \subseteq \Omega\ \mathit{and}\ |P| = x.$$

Applications

FFMSP belong to the class of ploblem know as *sequences consensus*.
Molecular biology applications:

- creating diagnostic probes for bacterial infections;
- discovering potential drug targets.

State of the art

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- C.C. Ribeiro, I. Rosseti, and R. Vallejos. Exploiting run time distributions to compare sequential and parallel stochastic local search algorithms. *Journal of Global Optimization*, 54:405–429, 2012

Metaheuristics

Pure metaheuristics:

- GRASP
- VNS

Hybrid metaheuristics:

- GRASP + Path-relinking
- VNS + Path-relinking
- GRASP + VNS + Path-relinking

GRASP

GRASP (Greedy Randomized Adaptive Search Procedure) is a multi-start metaheuristic, where each iteration consists of two phases.

algorithm $\texttt{GRASP}(f(\cdot), g(\cdot), \mathcal{N}, \texttt{Seed})$
s_{best}:=$\emptyset$; $f(s_{best})$:=$-\infty$;
while stopping criterion not satisfied$\rightarrow$
  s:=$\texttt{BuildGreedyRandomSolution}(\texttt{Seed}, g(\cdot))$;
  s:=$\texttt{LocalSearch}(s, f(\cdot), \mathcal{N})$;
  if $(f(s) > f(s_{best}))$ **then**
    s_{best}:=s;
  endif
endwhile
return(s_{best});
end $\texttt{GRASP}$

Construction phase

In a typical iteration, let S be a partial solution.
Let g_{min} and g_{max} be the smallest and the largest greedy values among the $|L|$ candidates, respectively, i.e.

$$g_{min} = \min_{e \in L} g(e), \quad g_{max} = \max_{e \in L} g(e).$$

A **R**estricted **C**andidate **L**ist is made up of all elements $e \in L$ with the best greedy values $g(e)$.

Random component: $e :=$`select`(RCL); $S := S \cup \{e\}$;

Adaptive component: greedy function values depend on the partial solution constructed so far.

Construction phase

For each position $j = 1, \ldots, m$ and for each $c \in \Sigma$ we compute

$$V_j(c) = \left| \{ i = 1, \ldots, n | s_j^i = c \} \right| .$$

To define the construction mechanism for the RCL, let

$$V_j^{\min} = \min_{c \in \Sigma} V_j(c), \quad V_j^{\max} = \max_{c \in \Sigma} V_j(c).$$

To build the RCL we have adopted a *value-based* (VB) mechanism: RCL is associated with a **parameter** $\alpha \in [0, 1]$ and a threshold value $\mu_j = V_j^{\min} + \alpha \cdot (V_j^{\max} - V_j^{\min})$:

$$\mathrm{RCL}_j = \{ c \in \Sigma \colon V_j(e) \leq \mu_j \}.$$

Construction phase

function GrRand(m, Σ, $\{V_j(c)\}_{j\in\{1,\ldots,m\}}^{c\in\Sigma}$, $V_j^{\min}$, $V_j^{\max}$, Seed)
for $j = 1$ **to** $m \rightarrow$
    RCL$_j$:=$\emptyset$; α:=Random([0, 1], Seed);
    $\mu := V_j^{\min} + \alpha \cdot (V_j^{\max} - V_j^{\min})$;
    for all $c \in \Sigma \rightarrow$
        if $(V_j(c) \leq \mu)$) **then**
            RCL$_j$:=RCL$_j \cup \{c\}$;
        endif
    endfor
    s_j:=Random(RCL$_j$, Seed);
endfor
return(s, $\{\text{RCL}_j\}_{j=1}^{m}$);
end GrRand

Construction phase

function $\texttt{GrRand}(m,\ \Sigma,\ \{V_j(c)\}_{j\in\{1,\dots,m\}}^{c\in\Sigma},\ V_j^{\min},\ V_j^{\max},\ \texttt{Seed})$

for $j = 1$ **to** $m \rightarrow$

  $\mathrm{RCL}_j := \emptyset;\ \alpha := \texttt{Random}([0,1],\ \texttt{Seed});$

  $\mu := V_j^{\min} + \alpha \cdot (V_j^{\max} - V_j^{\min});$

  for all $c \in \Sigma \rightarrow$

    if $(V_j(c) \le \mu))$ **then**

      $\mathrm{RCL}_j := \mathrm{RCL}_j \cup \{c\};$

    endif

  endfor

  $s_j := \texttt{Random}(\mathrm{RCL}_j,\ \texttt{Seed});$

endfor

return$(s,\ \{\mathrm{RCL}_j\}_{j=1}^{m});$

end $\texttt{GrRand}$

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    for all $c \in \Sigma \rightarrow$
        if $(V_j(c) \leq \mu))$ **then**
            $\mathrm{RCL}_j{:=}\mathrm{RCL}_j \cup \{c\}$;
        endif
    endfor
    $s_j{:=}\texttt{Random}(\mathrm{RCL}_j,\ \texttt{Seed})$;
endfor
return$(s,\ \{\mathrm{RCL}_j\}_{j=1}^{m})$;

end $\texttt{GrRand}$

Neighborhood

To define local search, one needs to specify a local neighborhood structure $N(s)$ of a solution s:

$$N(s) = \{\bar{s} | d_H(s, \bar{s}) = 1 \wedge (\forall j = 1, \ldots, n, s_j \neq \bar{s}_j \implies \bar{s}_j \in RCL_j)\}$$

Local search

```
function LocalSearch(m, s, f(·), {RCL_j}_{j=1}^m)
  max:=f(s); change:=.TRUE.;
  while (change)→
    change:=.FALSE.;
    for j = 1 to m→
        temp:=s_j;
        for all c ∈RCL_j→
            s_j:=c;
            if (f(s) > max) then
                max:=f(s); temp:=c; change:=.TRUE.; break;
            endif
        endfor
        s_j:=temp;
    endfor
  endwhile
  return(s);
end LocalSearch
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                max:=f(s); temp:=c; change:=.TRUE.; break;
            endif
        endfor
        s_j:=temp;
    endfor
  endwhile
  return(s);
end LocalSearch
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VNS

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$$N_k(s) = \{\bar{s} | d_H(s, \bar{s}) = k \wedge (\forall j = 1, \ldots, n, s_j \neq \bar{s}_j \implies \bar{s}_j \in RCL_j)\}$$

algorithm $\texttt{VNS}(m, \Sigma, f(\cdot), k_{max}, \texttt{Seed})$

$s_{best}{:=}\emptyset;\ f(s_{best}){:=}-\infty;$

while stopping criterion not satisfied$\rightarrow$

  $k{:=}1;\ s{:=}\texttt{BuildRand}(m, \Sigma, \texttt{Seed});$ /* pure randomly */

  while $(k \leq k_{max})\rightarrow$

    $s'{:=}\texttt{Random}(N_k(s), \texttt{Seed}, \{\mathrm{RCL}_j\}_{j=1}^{m});$

    $s''{:=}\texttt{locsearch}(m, s', f(\cdot), \{\mathrm{RCL}_j\}_{j=1}^{m});$

    if $(f(s'') > f(s))$ **then**

      $s{:=}s'';\ k{:=}1;$

      if $(f(s'') > f(s_{best}))$ **then** $s_{best}{:=}s'';$

      endif

    else $k{:=}k+1;$

    endif

  endwhile

endwhile

return$(s_{best});$

end $\texttt{VNS}$

Path-relinking

- It explores trajectories that connect high quality solutions.
- Path is generated by selecting modifications (moves) that introduce attributes of the guiding solution G in the initial solution I.
- At each step, all moves ($d(I, G)$) that incorporate attributes of the guiding solution are analyzed and best move is taken.

Path-relinking

algorithm `Path-relinking`$(m,\ f(\cdot), \mathtt{s}, \mathcal{E},$ `Seed`$)$

$\hat{\mathbf{s}}$:=`Random`$(\mathcal{E},$ `Seed`$)$;

$f^* := \max\{f(\mathbf{s}), f(\hat{\mathbf{s}})\}$; $\mathbf{s}^* := \arg\max\{f(\mathbf{s}), f(\hat{\mathbf{s}})\}$;

$\mathbf{s}' := \arg\min\{f(\mathbf{s}), f(\hat{\mathbf{s}})\}$; $\hat{\mathbf{s}}$:=$\mathbf{s}^*$;

$\Delta(\mathbf{s}', \hat{\mathbf{s}})$:=$\{i = 1, \ldots, m \mid \mathbf{s'}_i \neq \hat{\mathbf{s}}_i\}$;

while $(\Delta(\mathbf{s}', \hat{\mathbf{s}}) \neq \emptyset) \rightarrow$

    $i^* := \arg\max\{f(\mathbf{s}' \oplus i) \mid i \in \Delta(\mathbf{s}', \hat{\mathbf{s}})\}$;

    $\Delta(\mathbf{s}' \oplus i^*, \hat{\mathbf{s}}) := \Delta(\mathbf{s}', \hat{\mathbf{s}}) \setminus \{i^*\}$;

    $\mathbf{s}' := \mathbf{s}' \oplus i^*$;

    if $(f(\mathbf{s}') > f^*)$ **then**

        $f^* := f(\mathbf{s}')$; $\mathbf{s}^* := \mathbf{s}'$;

    endif;

endwhile;

return $(\mathbf{s}^*)$;

end `Path-relinking`;

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algorithm Path-relinking(m, $f(\cdot)$, s, $\mathcal{E}$, Seed)
 $\hat{\mathbf{s}}$:=Random($\mathcal{E}$, Seed);
 $f^* := \max\{f(\mathbf{s}), f(\hat{\mathbf{s}})\}$; $\mathbf{s}^* := \arg\max\{f(\mathbf{s}), f(\hat{\mathbf{s}})\}$;
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 endwhile;
 return $(\mathbf{s}^*)$;
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algorithm $\texttt{Path-relinking}(m,\ f(\cdot), \mathtt{s}, \mathcal{E},\ \texttt{Seed})$

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endwhile;

return $(\mathbf{s}^*)$;

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algorithm $\texttt{GRASP+PR}(t,\ m,\ \Sigma,\ f_t(\cdot),\ \{V_j(c)\}_{j\in\{1,\ldots,m\}}^{c\in\Sigma},\ \texttt{Seed},\ \texttt{MaxElite})$

$s_{best}{:=}\emptyset$; $f_t(s_{best}){:=}-\infty$; $\mathcal{E} := \emptyset$; $iter{:=}0$;

for $j = 1$ **to** $m \rightarrow$

  $V_j^{\min}{:=}\min_{c\in\Sigma} V_j(c)$; $V_j^{\max}{:=}\max_{c\in\Sigma} V_j(c)$;

while stopping criterion not satisfied$\rightarrow$

  $iter{:=}iter+1$;

  $[s, \{\mathrm{RCL}_j\}_{j=1}^{m}]{:=}\texttt{GrRand}(m,\ \Sigma,\ \{V_j(c)\}_{j\in\{1,\ldots,m\}}^{c\in\Sigma},\ V_j^{\min},\ V_j^{\max},\ \texttt{Seed})$;

  $s{:=}\texttt{LocalSearch}(t,\ m,\ s,\ f_t(\cdot),\ \{\mathrm{RCL}_j\}_{j=1}^{m})$;

  if $(iter \leq \texttt{MaxElite})$ **then**

    $\mathcal{E} := \mathcal{E} \cup \{s\}$;

    if $(f_t(s) > f_t(s_{best}))$ **then** $s_{best}{:=}s$;

  else

    $\overline{s}{:=}\texttt{Path-relinking}(t,\ m,\ f_t(\cdot),\ s,\ \mathcal{E},\ \texttt{Seed})$;

    $\texttt{AddToElite}(\mathcal{E}, \overline{s})$;

    if $(f_t(\overline{s}) > f_t(s_{best}))$ **then** $s_{best}{:=}\overline{s}$;

return(s_{best});

end $\texttt{GRASP+PR}$

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      $\texttt{AddToElite}(\mathcal{E}, \overline{s});$

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return$(s_{best});$

end $\texttt{GRASP+PR}$

algorithm GRASP+PR(t, m, Σ, $f_t(\cdot)$, $\{V_j(c)\}_{j\in\{1,\ldots,m\}}^{c\in\Sigma}$, Seed, MaxElite)
s_{best}:=$\emptyset$; $f_t(s_{best})$:=$-\infty$; $\mathcal{E} := \emptyset$; $iter$:=0;
for $j = 1$ **to** $m\rightarrow$
  $V_j^{\min}$:=$\min_{c\in\Sigma} V_j(c)$; $V_j^{\max}$:=$\max_{c\in\Sigma} V_j(c)$;
while stopping criterion not satisfied$\rightarrow$
  $iter$:=$iter + 1$;
  $[s, \{\mathrm{RCL}_j\}_{j=1}^{m}]$:=GrRand($m$, Σ, $\{V_j(c)\}_{j\in\{1,\ldots,m\}}^{c\in\Sigma}$, $V_j^{\min}$, $V_j^{\max}$, Seed);
  s:=LocalSearch(t, m, s, $f_t(\cdot)$, $\{\mathrm{RCL}_j\}_{j=1}^{m}$);
  if ($iter \leq$ MaxElite) **then**
    $\mathcal{E} := \mathcal{E} \cup \{s\}$;
    if ($f_t(s) > f_t(s_{best})$) **then** s_{best}:=s;
  else
    $\overline{s}$:=Path-relinking(t, m, $f_t(\cdot)$, s, $\mathcal{E}$, Seed);
    AddToElite($\mathcal{E}$, $\overline{s}$);
    if ($f_t(\overline{s}) > f_t(s_{best})$) **then** s_{best}:=$\overline{s}$;
return(s_{best});
end GRASP+PR

algorithm $\texttt{GRASP+PR}(t,\ m,\ \Sigma,\ f_t(\cdot),\ \{V_j(c)\}_{j\in\{1,\dots,m\}}^{c\in\Sigma},\ \texttt{Seed},\ \texttt{MaxElite})$

$s_{best}{:=}\emptyset;\ f_t(s_{best}){:=}-\infty;\ \mathcal{E} := \emptyset;\ iter{:=}0;$

for $j = 1$ **to** $m \rightarrow$

  $V_j^{\min}{:=}\min_{c\in\Sigma} V_j(c);\ V_j^{\max}{:=}\max_{c\in\Sigma} V_j(c);$

while stopping criterion not satisfied$\rightarrow$

  $iter{:=}iter + 1;$

  $[s, \{\mathrm{RCL}_j\}_{j=1}^{m}]{:=}\texttt{GrRand}(m,\ \Sigma,\ \{V_j(c)\}_{j\in\{1,\dots,m\}}^{c\in\Sigma},\ V_j^{\min},\ V_j^{\max},\ \texttt{Seed});$

  $s{:=}\texttt{LocalSearch}(t,\ m,\ s,\ f_t(\cdot),\ \{\mathrm{RCL}_j\}_{j=1}^{m});$

  if $(iter \leq \texttt{MaxElite})$ **then**

    $\mathcal{E} := \mathcal{E} \cup \{s\};$

    if $(f_t(s) > f_t(s_{best}))$ **then** $s_{best}{:=}s;$

  else

    $\overline{s}{:=}\texttt{Path-relinking}(t,\ m,\ f_t(\cdot),\ s,\ \mathcal{E},\ \texttt{Seed});$

    $\texttt{AddToElite}(\mathcal{E}, \overline{s});$

    if $(f_t(\overline{s}) > f_t(s_{best}))$ **then** $s_{best}{:=}\overline{s};$

return$(s_{best});$

end $\texttt{GRASP+PR}$

Further hybrids

- GRASP+VNS: VNS applied as local search;
- VNS+PR: Path-relinking applied as intensification strategy;
- GRASP+VNS+PR: VNS applied as local search and Path-relinking as intensification strategy.

Compiler: *cc (GCC) 4.1.3 20070929 (prerelease) (Ubuntu 4.1.2-16ubuntu2*
Hardware: *Intel Core i7 Quad core @ 2.67 GHz RAM 6GB*
OS: *Linux (Ubuntu 11.10)*

- m ranges from 300 to 800;
- n ranges from 100 to 200;
- threshold t varies from $75\%m$ to $85\%m$;
- 100 random istances for each problem size;
- $k_{max} = 30$
- `MaxElite` $= 10$
- in Path-relinking a solution s is *sufficiently different* if $d_H(s, \epsilon) \geq \frac{m}{2}$, for all $\epsilon \in \mathcal{E}$.

n, m, t	GRASP		VNS		VNS+PR	
	z	Time	z	Time	z	Time
$100, 300, 0.75$	**100**	1.37	94.47	72.45	**100**	7.44
$100, 300, 0.80$	67.86	1.67	19.98	71.02	48.58	77.43
$100, 300, 0.85$	3.56	1.72	1.12	37.65	3.53	44.19
$100, 600, 0.75$	**100**	1.56	91.78	278.94	**100**	31.91
$100, 600, 0.80$	65.35	2.31	8.51	264.66	20.72	295.49
$100, 600, 0.85$	1.21	1.28	0.04	152.64	0.91	186.71
$100, 800, 0.75$	**100**	1.84	87.36	549.60	**100**	63.00
$100, 800, 0.80$	67.76	1.42	4.41	450.63	10.94	527.76
$100, 800, 0.85$	0.30	2.98	0.66	273.98	0.63	329.48
$200, 300, 0.75$	197.78	1.22	180.08	135.61	**200**	47.91
$200, 300, 0.80$	76.50	1.39	36.71	150.51	66.81	160.37
$200, 300, 0.85$	2.83	1.59	2.16	86.60	4.62	104.13
$200, 600, 0.75$	**200**	1.94	178.11	545.50	**200**	75.43
$200, 600, 0.80$	62.80	1.63	11.93	588.35	33.41	625.66
$200, 600, 0.85$	0.98	1.79	0.71	305.29	0.96	369.29
$200, 800, 0.75$	**200**	1.04	175.06	947.80	**200**	193.30
$200, 800, 0.80$	44.66	1.75	6.37	987.35	17.12	1102.47
$200, 800, 0.85$	0.86	1.55	0.15	544.21	0.49	659.02

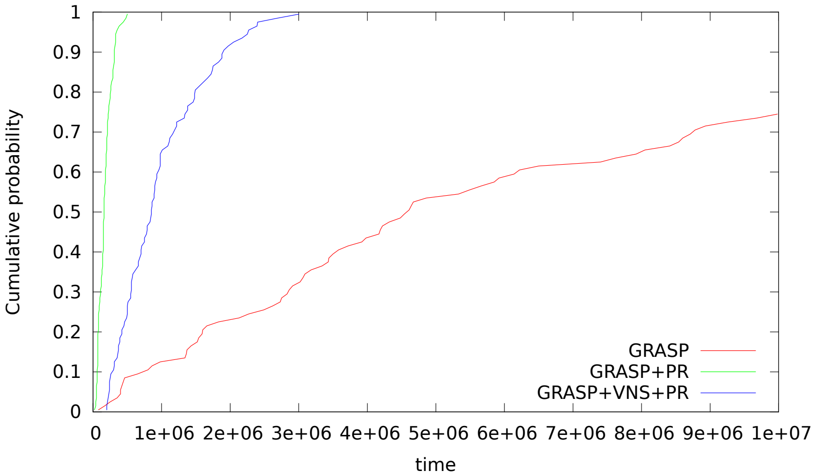
n, m, t	GRASP		GRASP+PR		GRASP+VNS+PR	
	z	Time	z	Time	z	Time
$100, 300, 0.75$	**100**	1.37	**100**	1.41	**100**	1.71
$100, 300, 0.80$	67.86	1.67	76.17	3.21	**76.68**	33.28
$100, 300, 0.85$	3.56	1.72	10.17	4.17	**12.23**	31.36
$100, 600, 0.75$	**100**	1.56	**100**	1.89	**100**	1.11
$100, 600, 0.80$	65.35	2.31	78.83	11.77	**80.47**	122.65
$100, 600, 0.85$	1.21	1.28	3.58	11.07	**4.36**	91.87
$100, 800, 0.75$	**100**	1.84	**100**	1.34	**100**	2.48
$100, 800, 0.80$	67.76	1.42	80.37	21.10	**82.30**	251.26
$100, 800, 0.85$	0.30	2.98	0.97	31.45	**2.51**	148.98
$200, 300, 0.75$	197.78	1.22	**200**	1.85	**200**	3.70
$200, 300, 0.80$	76.50	1.39	93.70	6.52	**94.45**	65.44
$200, 300, 0.85$	2.83	1.59	9.26	8.59	**11.12**	68.20
$200, 600, 0.75$	**200**	1.94	**200**	1.61	**200**	3.39
$200, 600, 0.80$	62.80	1.63	83.91	24.91	**86.17**	274.93
$200, 600, 0.85$	0.98	1.79	1.51	31.22	**2.38**	174.73
$200, 800, 0.75$	**200**	1.04	**200**	1.33	**200**	1.61
$200, 800, 0.80$	44.66	1.75	71.28	43.63	**72.44**	519.59
$200, 800, 0.85$	0.86	1.55	1.93	59.20	**3.71**	311.81

n, m, t	GRASP	GRASP+PR	GRASP+VNS+PR	VNS	VNS+PR
100, 300, 0.75	**100**	**100**	**100**	94	**100**
100, 300, 0.8	71.07	**79.61**	78.12	23.43	49.54
100, 300, 0.85	6.41	**13.18**	11.86	1.02	3.27
100, 600, 0.75	**100**	**100**	**100**	91.79	**100**
100, 600, 0.8	70.24	**80.13**	78.05	6.38	11.29
100, 600, 0.85	2.73	**4.98**	4.48	0.03	0.12
100, 800, 0.75	**100**	**100**	**100**	85.18	**100**
100, 800, 0.8	70.07	**82.64**	79.45	3.71	8.42
100, 800, 0.85	1.17	**1.84**	1.65	0	0.03
200, 300, 0.75	199.81	**200**	**200**	179.34	**200**
200, 300, 0.8	81.75	**100**	95.11	34.71	61.67
200, 300, 0.85	4.82	**11.90**	11.03	2.32	3.70
200, 600, 0.75	**200**	**200**	**200**	172.41	**200**
200, 600, 0.8	66.23	**88.49**	80.31	10.25	19.10
200, 600, 0.85	1.03	**2.42**	1.73	0.09	0.97
200, 800, 0.75	**200**	**200**	**200**	164.01	194.45
200, 800, 0.8	49.87	**73.08**	62.36	4.23	8.17
200, 800, 0.85	0.08	**0.21**	0.17	0.06	0.85

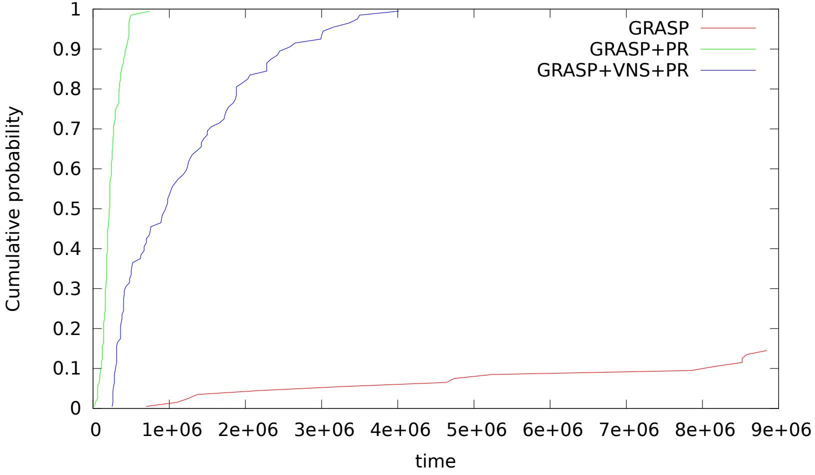
Time-to-target

- Target value $\hat{z}$;
- 100 different random instances;
- to the i^{th} sorted running time (t_i) we associate a probability $p_i = \frac{i-1/2}{100}$;
- plot the points $z_i = (t_i, p_i)$ for $i = 1, \ldots, 100$.

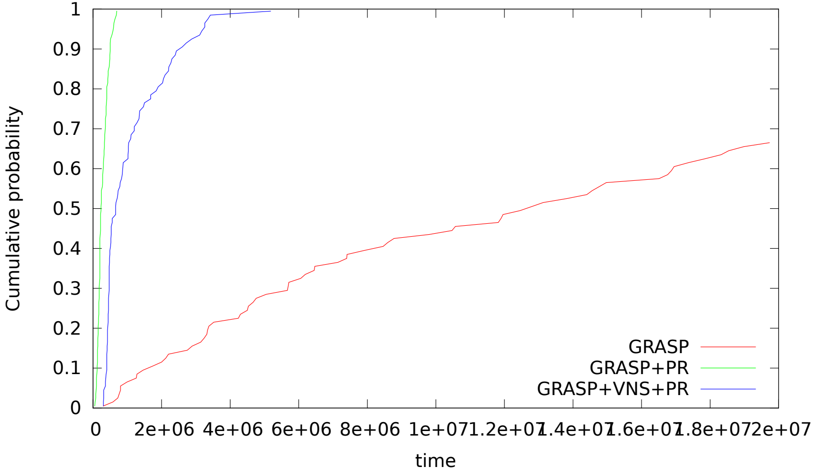
$n = 100, m = 300, t = 240, \hat{z} = 70$



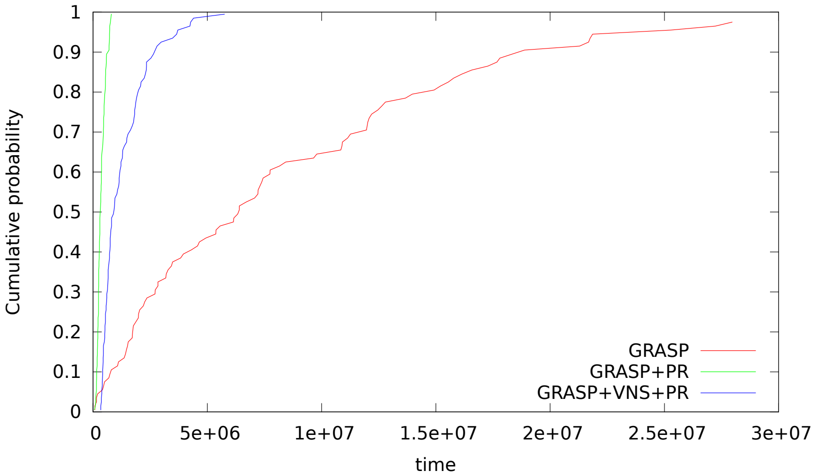
$n = 100, m = 300, t = 252, \hat{z} = 12$



$n = 200, m = 300, t = 240, \hat{z} = 80$



$n = 300, m = 300, t = 240, \hat{z} = 84$



Future work

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THANK YOU!