A Heuristic for Nonlinear Global Optimization

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A heuristic for nonlinear global optimization

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Global optimization

Motivation: estimation of econometric models

- (Conditional) Maximum Likelihood estimation of MEV models
- More advanced models:
  - continuous and discrete mixtures of MEV models
  - estimation with panel data
  - latent classes
  - latent variables
  - discrete-continuous models
  - etc...

Global optimization

Objective: identify the global minimum of

$$\min_{x \in \mathbb{R}^n} f(x),$$

where

- $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable.
- No special structure is assumed on f.

Literature

Local nonlinear optimization:

- Main focus:
  - global convergence
  - towards a local minimum
  - with fast local convergence.
- Vast literature
- Efficient algorithms
- Softwares

Literature

Global nonlinear optimization: exact approaches

- Real algebraic geometry (representation of polynomials, semidefinite programming)
- Interval arithmetic
- Branch & Bound
- DC - difference of convex functions

Literature

Global nonlinear optimization: heuristics

- Usually hybrid between derivative-free methods and heuristics from discrete optimization. Examples:

- Glover (1994) Tabu + scatter search
- Franze and Speciale (2001) Tabu + pattern search
- Hedar and Fukushima (2004) Sim. annealing + pattern
- Hedar and Fukushima (2006) Tabu + direct search
- Mladenovic et al. (2006) Variable Neighborhood search (VNS)

Our heuristic

Framework: VNS

Ingredients:

1. Local search

$$(\text{SUCCESS}, y^*) \leftarrow \text{LS}(y_1, \ell_{\text{max}}, \mathcal{L}),$$

where

- y_1 is the starting point
- ℓ_{max} is the maximum number of iterations
- $\mathcal{L}$ is the set of already visited local optima
- Algorithm: trust region

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Our heuristic

1. Local search

$$(\text{SUCCESS}, y^*) \leftarrow \text{LS}(y_1, \ell_{\text{max}}, \mathcal{L}),$$

- If $\mathcal{L} \neq \emptyset$, LS may be interrupted prematurely
- If $\mathcal{L} = \emptyset$, LS runs toward convergence
- If local minimum identified, SUCCESS=true

Our heuristic

2. Neighborhood structure
   - Neighborhoods: $\mathcal{N}_k(x)$, $k = 1, \ldots, n_{\text{max}}$
   - Nested structure: $\mathcal{N}_k(x) \subset \mathcal{N}_{k+1}(x) \subseteq \mathbb{R}^n$, for each k
   - Neighbors generation

$$(z_1, z_2, \ldots, z_p) = \text{NEIGHBORS}(x, k).$$

   - Typically, $n_{\text{max}} = 5$ and $p = 5$.

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The VNS framework

Initialization x_1^* local minimum of f

- Cold start: run LS once
- Warm start: run LS from randomly generated starting points

Stopping criteria Interrupt if

1. $k > n_{\text{max}}$: the last neighborhood has been unsuccessfully investigated
2. CPU time $\geq t_{\text{max}}$, typ. 30 minutes (18K seconds).
3. Number of function evaluations $\geq$ eval$_{\text{max}}$, typ. 10^5.

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The VNS framework

Main loop Steps:

1. Generate neighbors of x^k_{best}:

$$(z_1, z_2, \ldots, z_p) = \text{NEIGHBORS}(x^k_{\text{best}}, k). \quad (1)$$

2. Apply the p local search procedures:

$$(\text{SUCCESS}_j, y^*_j) \leftarrow \text{LS}(z_j, \ell_{\text{large}}, \mathcal{L}). \quad (2)$$

3. If SUCCESS_j =FALSE, for $j = 1, \ldots, p$, we set $k = k + 1$ and proceed to the next iteration.

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The VNS framework

Main loop Steps (ctd):

4. Otherwise,

$$\mathcal{L} = \mathcal{L} \cup \{y_j^*\}. \tag{3}$$

   for each j such that SUCCESS$_j$ =TRUE

5. Define x_{best}^{k+1}

$$f(x_{\text{best}}^{k+1}) \leq f(x), \text{ for each } x \in \mathcal{L}. \tag{4}$$

6. If $x_{\text{best}}^{k+1} = x_{\text{best}}^{k}$, no improvement. We set $k = k + 1$ and proceed to the next iteration.

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The VNS framework

Main loop Steps (ctd):

7. Otherwise, we have found a new candidate for the global optimum. The neighborhood structure is reset, we set $k = 1$ and proceed to the next iteration.

Output The output is the best solution found during the algorithm, that is x^k_{best}.

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Local search

- Classical trust region method with quasi-newton update
- Key feature: premature interruption
- Three criteria: we check that
  1. the algorithm does not get too close to an already identified local minimum.
  2. the gradient norm is not too small when the value of the objective function is far from the best.
  3. a significant reduction in the objective function is achieved.

Neighborhoods

The key idea: analyze the curvature of f at x

- Let $v_1, \ldots, v_n$ be the (normalized) eigenvectors of H
- Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues.
- Define direction $w_1, \ldots, w_{2n}$, where $w_i = v_i$ if $i \leq n$, and $w_i = -v_i$ otherwise.
- Size of the neighborhood: $d_1 = 1$, $d_k = 1.5 d_{k-1}$, $k = 2, \ldots$.

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Neighborhoods

- Neighbors:

$$z_j = x + \alpha d_k w_i, \quad j = 1, \ldots, p, \tag{5}$$

  where
  - α is randomly drawn $U[0.75, 1]$
  - i is a selected index
- Selection of w_i:
  - Prefer directions where the curvature is larger
  - Motivation: better potential to jump in the next valley

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Neighborhoods: selection of w_i

$$P(w_i) = P(-w_i) = \frac{e^{\beta \frac{|\lambda_i|}{d_k}}}{2 \sum_{j=1}^{n} e^{\beta \frac{|\lambda_j|}{d_k}}}.$$

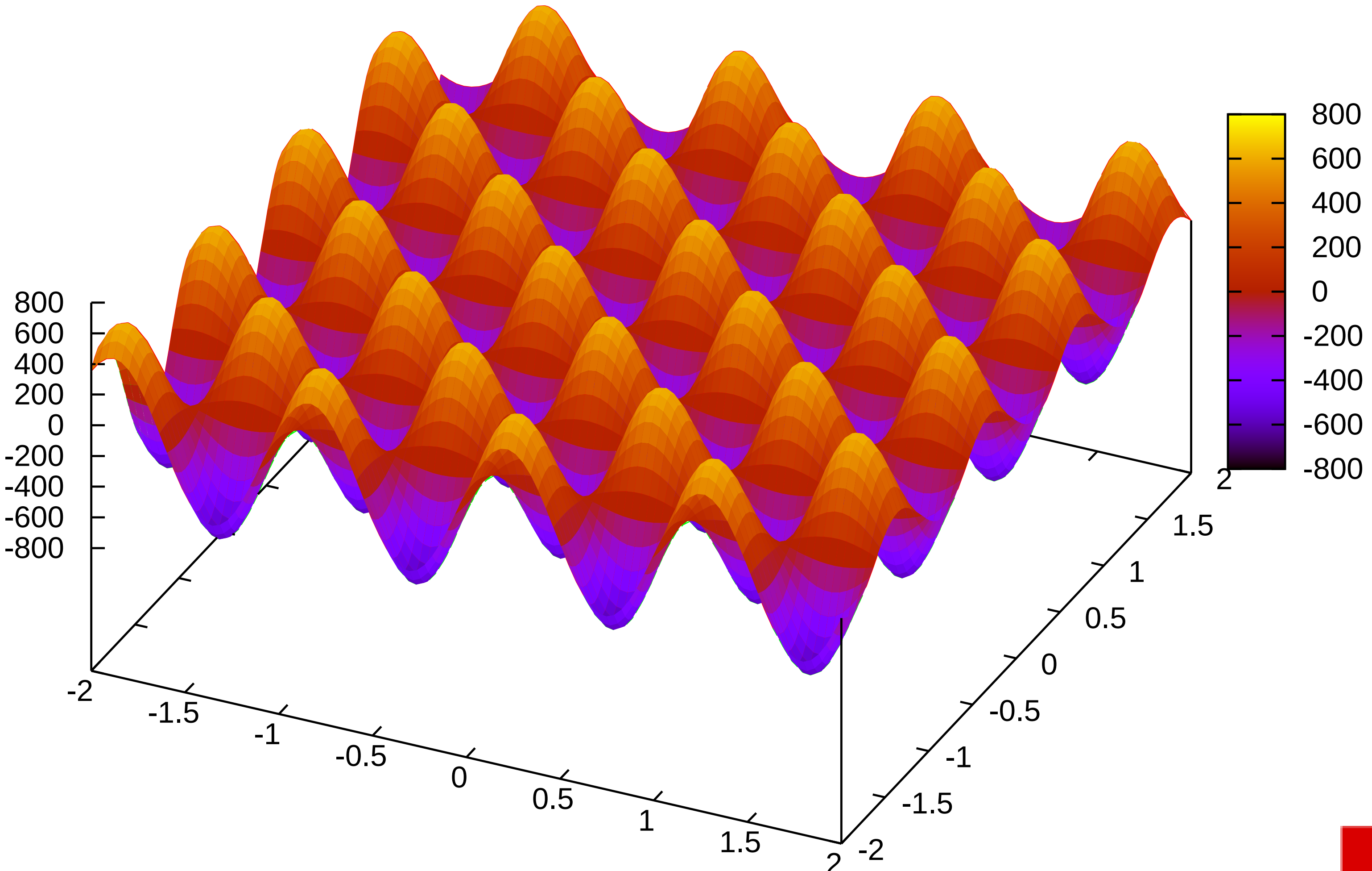
- In large neighborhoods (d_k large), curvature is less relevant and probabilities are more balanced.
- We tried $\beta = 0.05$ and $\beta = 0$.
- The same w_i can be selected more than once
- The random step α is designed to generate different neighbors in this case

Numerical results

- 25 problems from the literature
- Dimension from 2 to 100
- Most with several local minima
- Some with “crowded” local minima
- Measures of performance:
  1. Percentage of success (i.e. identification of the global optimum) on 100 runs
  2. Average number of function evaluations for successful runs

Shubert function

$$(\sum_{j=1}^{5} j\cos((j+1)x_1+j))(\sum_{j=1}^{5} j\cos((j+1)x_2+j))$$



Numerical results

Competition:

1. Direct Search Simulated Annealing (DSSA) Hedar & Fukushima (2002).
2. Continuous Hybrid Algorithm (CHA) Chelouah & Siarry (2003).
3. Simulated Annealing Heuristic Pattern Search (SAHPS) Hedar & Fukushima (2004).
4. Directed Tabu Search (DTS) Hedar & Fukushima (2006) .
5. General variable neighborhood search (GVNS) Mladenovic et al. (2006)

Numerical results: success rate

Problem	VNS	CHA	DSSA	DTS	SAHPS	GVNS
RC	100	100	100	100	100	100
ES	100	100	93	82	96	
RT	84	100	100		100	
SH	78	100	94	92	86	100
R_2	100	100	100	100	100	100
Z_2	100	100	100	100	100	
DJ	100	100	100	100	100	
$H_{3,4}$	100	100	100	100	95	100
$S_{4,5}$	100	85	81	75	48	100
$S_{4,7}$	100	85	84	65	57	
$S_{4,10}$	100	85	77	52	48	100

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Numerical results: success rate

Problem	VNS	CHA	DSSA	DTS	SAHPS	GVNS
R_5	100	100	100	85	91	
Z_5	100	100	100	100	100	
$H_{6,4}$	100	100	92	83	72	100
R_{10}	100	83	100	85	87	100
Z_{10}	100	100	100	100	100	
HM	100		100			
GR_6	100		90			
GR_{10}	100					100
CV	100		100			
DX	100		100			
MG	100					100

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Numerical results: success rate

Problem	VNS	CHA	DSSA	DTS	SAHPS	GVNS
R_{50}	100	79		100		
Z_{50}	100	100		0		
R_{100}	100	72		0		

- Excellent success rate on these problems
- Best competitor: GVNS (Mladenovic et al, 2006)

Performance Profile

→ Performance Profile proposed by Dolan and Moré (2002)

Algorithms	*Problems*									
Method A	20	10	**	10	**	20	10	15	25	**
Method B	10	30	70	60	70	80	60	75	**	**

Performance Profile

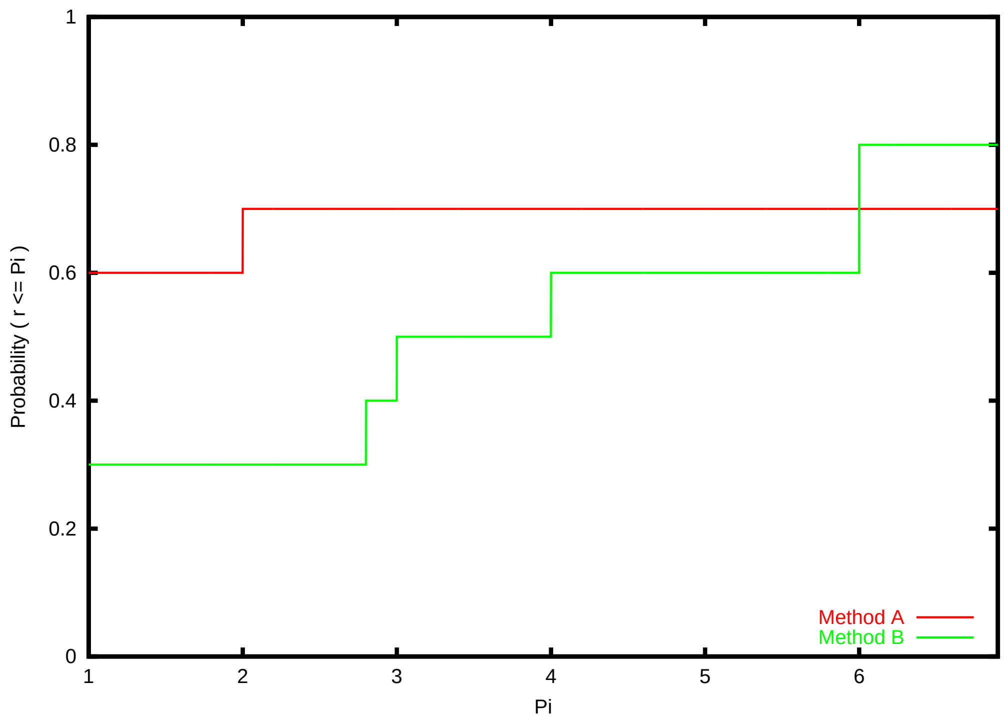
$\longrightarrow$ Performance Profile proposed by Dolan and Moré (2002)

Algorithms	*Problems*									
Method A	2	1	r_{fail}	1	r_{fail}	1	1	1	1	r_{fail}
Method B	1	3	1	6	1	4	6	5	r_{fail}	r_{fail}

Performance Profile

$\rightarrow$ Performance Profile proposed by Dolan and Moré (2002)

Algorithms	*Problems*									
Method A	2	1	r_{fail}	1	r_{fail}	1	1	1	1	r_{fail}
Method B	1	3	1	6	1	4	6	5	r_{fail}	r_{fail}



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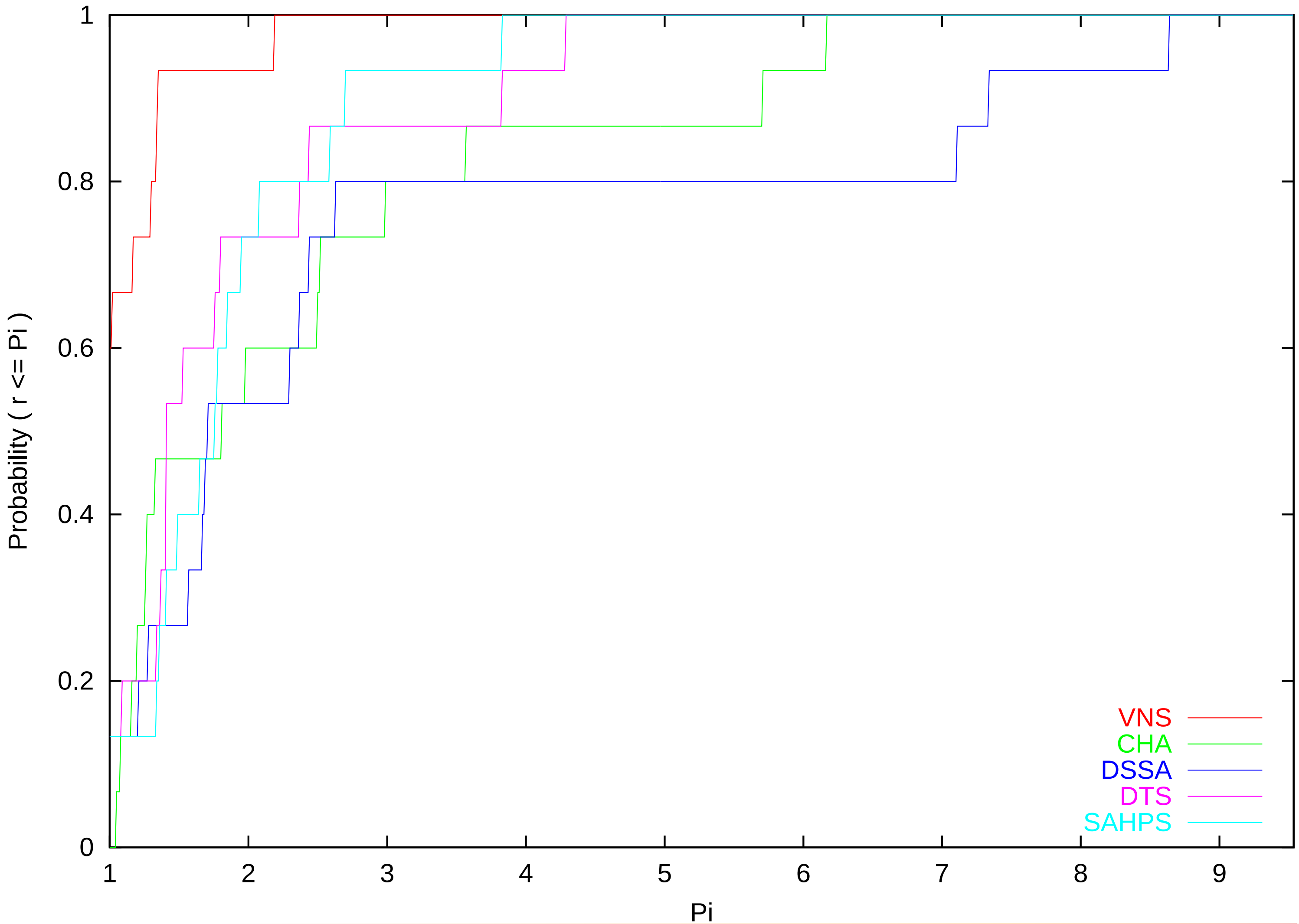
Numerical results: efficiency

Number of function evaluations (4 competitors)



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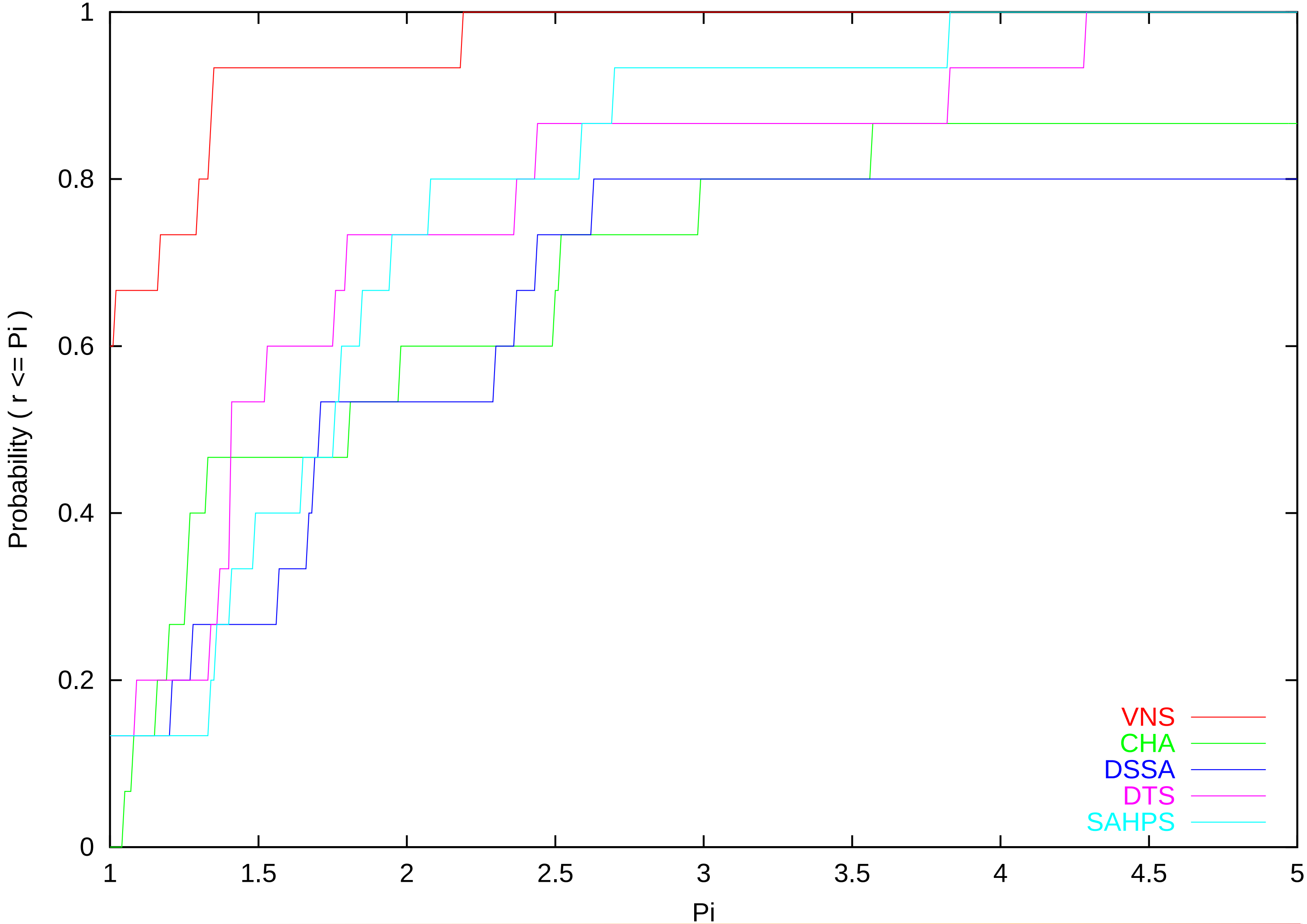
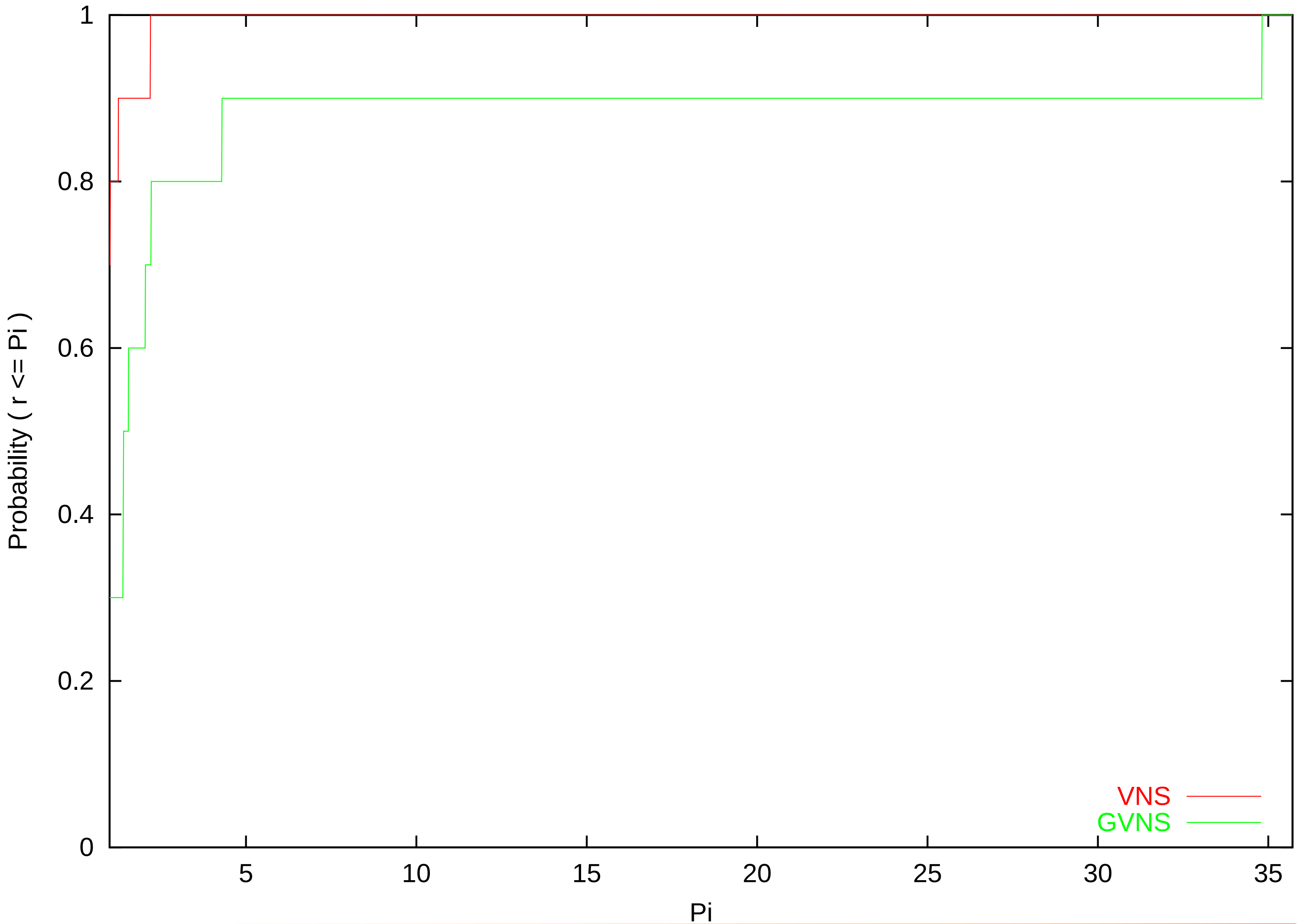
Numerical results: efficiency

Number of function evaluations (zoom)



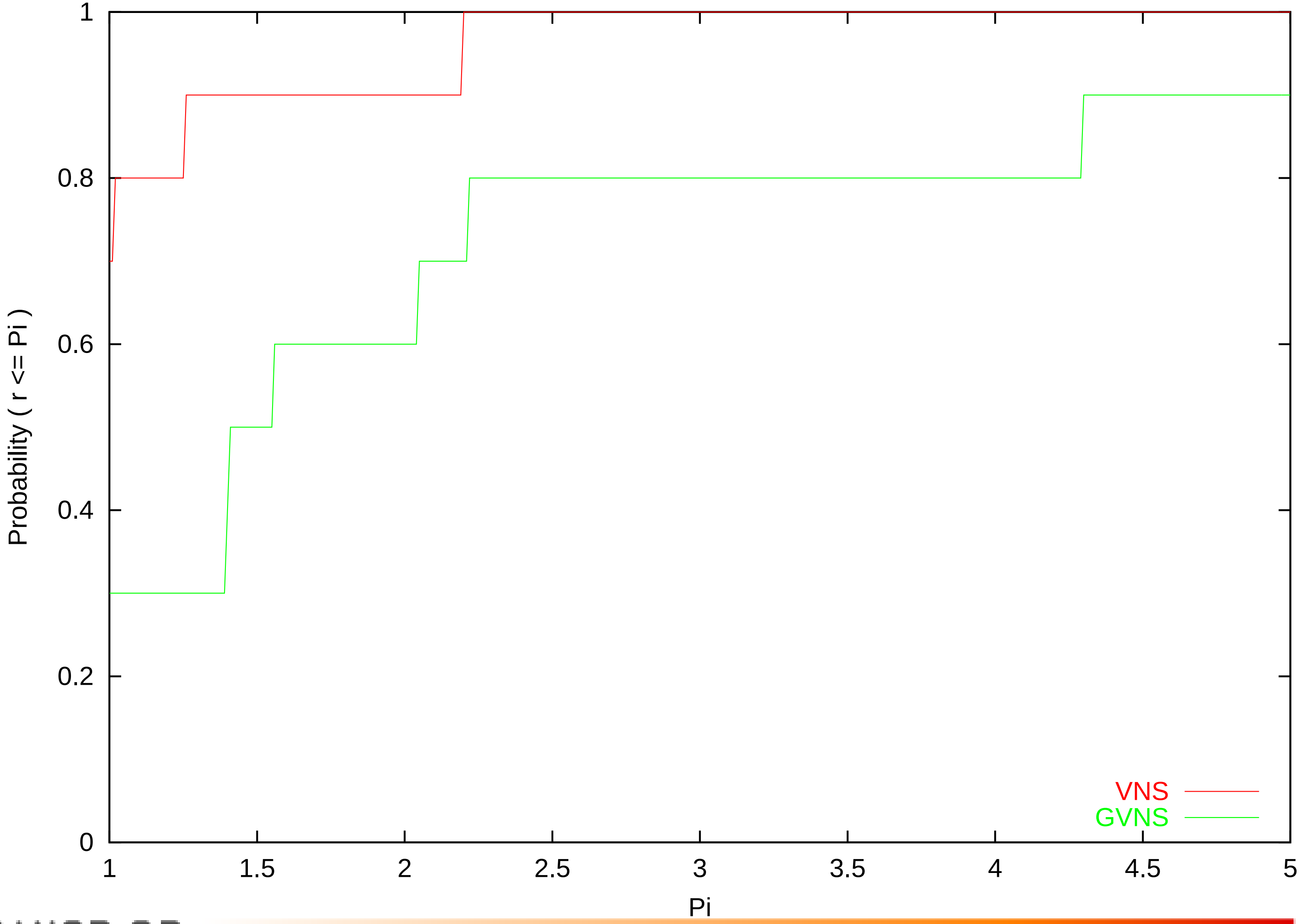
Numerical results: efficiency

Number of function evaluations (GVNS)



Numerical results: efficiency

Number of function evaluations (zoom)



Conclusions

- Use of state of the art methods from
  - nonlinear optimization: TR + Q-Newton
  - discrete optimization: VNS
- Two new ingredients:
  - Premature stop of LS to spare computational effort
  - Exploits curvature for smart coverage
- Numerical results consistent with the algorithm design