A Collocation Solver for Singular Boundary Value Problems

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Problem Class

$$z'(t) = \underbrace{\frac{M(t)}{t} z(t) + f(t, z(t))}_{=:F(t,z(t))}, \quad t \in (0, 1],$$

$$B_a z(0) + B_b z(1) = \beta.$$

Remark: 2[nd] order problems of the form

$$y''(t) = \frac{A_1(t)}{t} y'(t) + \frac{A_0(t)}{t^2} y(t) + f(t, y(t))$$

can be transformed to the first order form by setting

$$z(t) := (y(t), t y'(t)).$$

Applications:

- chemical reactor theory
- physics — theory of lasers, computational material science
- mechanics — buckling of (spherical) shells
- ecology — run-up of avalanches

The Solution Method

- Collocation at **equidistant** or **Gaussian** points.

- New global error estimate
  in mesh points + collocation points:
  Defect Correction Principle!

- Equidistribution of the global error.

Motivation

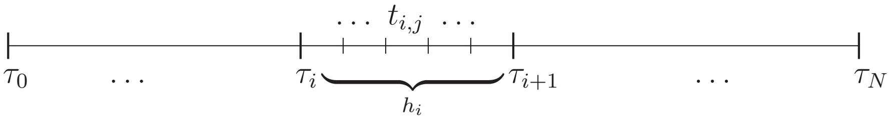
- Order reductions for singular problems occur for various standard methods:
  - explicit Runge-Kutta methods
  - Multistep methods
  - Acceleration techniques (IDeC, extrapolation)

    for general class of BVPs
- Shooting + IDeC based on the backward Euler method works, but:

  Only for a restricted class of BVPs!
- Estimates of the local error do not work for singular problems in general,

  e.g. when using:
  - standard three-point discretization for 2^{nd} order problems
  - explicit Runge-Kutta pairs

Collocation



$$p'(t_{i,j}) = F(t_{i,j}, p(t_{i,j})),$$
$$j = 1, \dots, m,\ i = 0, \dots, N-1,$$
$$B_a p(0) + B_b p(1) = \beta.$$

The **stage order is retained**, but there is **no superconvergence** in general.

However, the order reduction is actually not observed for most singular problems $\Longrightarrow$

- even number of equidistant (interior) collocation points .... **default**
- Gaussian points .... **optional**

Interior collocation points:

- No evaluation at the singular point $t = 0$
- Error estimate requires $t_{i,m} \neq \tau_{i+1}$

Global Error Estimation

- We construct a **neighboring problem** using the **Defect Correction Principle**.
- Then we solve for $j = 1, \ldots, m+1$, $i = 0, \ldots, N-1$, the backward Euler schemes

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j},$$
$$B_a \pi_{0,0} + B_b \pi_{N-1,m+1} = \beta,$$

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F(t_{i,j}, \xi_{i,j}),$$
$$B_a \xi_{0,0} + B_b \xi_{N-1,m+1} = \beta,$$

where

$$t_{i,m+1} := \tau_{i+1}$$

denotes the endpoint of each interval.

The estimate for the global error is given by

$$\mathcal{E}_{i,j} := \pi_{i,j} - \xi_{i,j}.$$

Global Error Estimation (2)

The defect is chosen as

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \\ - \sum_{k=1}^{m+1} \alpha_{j,k} F(t_{i,k}, p(t_{i,k})).$$

Here, the $\alpha_{j,k}$ define a quadrature rule,

$$\frac{1}{t_{i,j}-t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(\tau)\, d\tau = \sum_{k=1}^{m+1} \alpha_{j,k} \varphi(t_{i,k}) + O(h_i^{m+1}).$$

Theorem: For regular problems and collocation at an even number of interior points, this estimate is asymptotically correct,

$$|(p(t_{i,j}) - z(t_{i,j})) - (\pi_{i,j} - \xi_{i,j})| = O(h_i^{m+1}), \\ j = 0, \ldots, m+1,\ i = 0, \ldots, N-1.$$

Proof: Auzinger, Koch, Weinmüller (2001).

Adaptive Mesh Selection

Monitor function $\Theta_{i,j}$ based on our error estimate,

$$\mathcal{E}_{i,j} := \pi_{i,j} - \xi_{i,j},$$
$$\Theta_{i,j} := \sqrt[m]{|\mathcal{E}_{i,j}|}.$$

Remark: Actually, a smoothed version of $\Theta_{i,j}$ is used.

$(\bar{\tau}_0, \ldots, \bar{\tau}_{\bar{N}})$ ... grid aiming at the equidistribution of the integral of the monitor function on the interval $[0, 1]$:

$$I := \int_0^1 \Theta(s)\, ds := \sum_{i,j} \frac{\Theta_{i,j} + \Theta_{i,j-1}}{2}(t_{i,j} - t_{i,j-1}),$$

$$\int_{\bar{\tau}_i}^{\bar{\tau}_{i+1}} \Theta(s)\, ds = \frac{I}{\bar{N}}, \; i = 0, \ldots, \bar{N} - 1.$$

Damped Newton Iteration

Let

$$x := x_{i,j},\ j = 1, \ldots, m+1,\ i = 0, \ldots, N-1$$

be the vector of the coefficients of the collocation solution w.r.t. a basis of piecewise polynomial functions,

$$p(t) = \sum_{j=1}^{m+1} x_{i,j}\, \varphi_j \left(\frac{t - \tau_i}{h_i} \right),\ t \in [\tau_i, \tau_{i+1}],$$

e. g. Lagrange basis, Runge-Kutta basis.

n-th approximation $x^{(n)}$:

$$x^{(n)} = x^{(n-1)} + \lambda^{(n)} \Delta x^{(n)},$$

$\Delta x^{(n)}$ . . . . classical Newton increment

$\lambda^{(n)}$ . . . . damping factor

See Deuflhard, Hohmann (1995).

Example

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} z(t) - \begin{pmatrix} 0 \\ t z_1^5(t) \end{pmatrix},$$

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} z(0) + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} z(1) = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}.$$

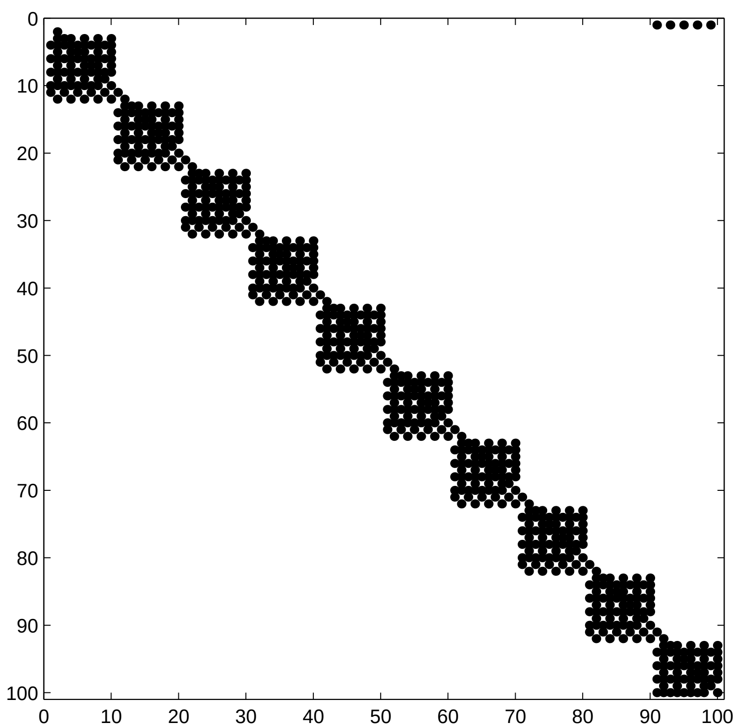
Exact solution:

$$z(t) = (z_1(t), z_2(t))^T = \left(\frac{1}{\sqrt{1+t^2/3}}, -\frac{t^2}{3\sqrt{(1+t^2/3)^3}} \right)^T.$$

n	$\mathrm{res}^{(n)}$	$\lvert\Delta x^{(n)}\rvert$	$p^{(n)}$	$\lambda^{(n)}$
1	6.34e+01	1.88e+00		0.500
2	3.17e+01	9.35e−01	−0.19	0.125
3	2.77e+01	1.07e+00	−3.02	0.250
4	2.08e+01	7.17e−01	1.70	0.500
5	1.04e+01	3.64e−01	2.51	1.000
6	3.94e−01	6.65e−02	1.01	1.000
7	4.01e−02	1.20e−02	2.30	1.000
8	9.40e−04	2.38e−04	1.92	1.000
9	4.23e−07	1.25e−07	2.01	1.000
10	1.07e−13	3.25e−14		1.000

Conditioning of the Jacobian

The nonlinear system of equations for $x = x_{i,j}$ leads to a Newton iteration with a Jacobian with the following sparse structure:



Conditioning (2)

Bad scaling $\Longrightarrow$ the condition number grows quadratically with the dimension.

Remedy: Preconditioner restores linear growth,

$$A = \begin{pmatrix} \frac{1}{h_1} I_n & & & & & & \\ & I_{mn} & & & & & \\ & & \frac{1}{h_1} I_n & & & & \\ & & & I_{mn} & & & \\ & & & & \frac{1}{h_2} I_n & & \\ & & & & & \ddots & \\ & & & & & & I_{mn} \end{pmatrix}.$$

N	cond_1	p_1	cond_2	p_2
4	5.13e+02		1.91e+03	
8	7.50e+02	0.54	5.54e+03	1.53
16	1.22e+03	0.70	1.80e+04	1.69
32	2.17e+03	0.82	6.37e+04	1.82
64	4.08e+03	0.90	2.38e+05	1.90
128	7.88e+03	0.95	9.22e+05	1.94
256	1.55e+04	0.97	3.62e+06	1.97
512	3.07e+04	0.98	1.43e+07	1.98
1024	6.11e+04	0.99	5.71e+07	1.99

Influence on the maximal attainable accuracy!

Choice of the Basis

The choice of the polynomial basis φ_j also has an important influence on the maximal attainable accuracy of the collocation solution.

Let

$$0 < \rho_1 < \cdots \rho_m < 1.$$

Lagrange basis:

$$\varphi_j(0) = \delta_{j,1}, \ \ \varphi_j(\rho_i) = \delta_{j,i+1}.$$

Runge-Kutta basis:

$$\varphi_j(0) = \delta_{j,1}, \ \ \varphi_j'(\rho_i) = \delta_{j,i+1}.$$

N	$m = 4$, RK	$m = 4$, La	$m = 6$, RK	$m = 6$, La
16	1.18e+08	1.18e+08	1.89e+04	1.88e+04
32	7.41e+06	7.41e+06	2.98e+02	1.37e+02
64	4.63e+05	4.63e+05	2.36e+00	4.36e+02
128	2.89e+04	2.87e+04	4.00e+00	8.79e+02
256	1.81e+03	1.31e+03	1.52e+00	1.75e+03
512	1.12e+02	8.95e+02	4.06e+00	3.50e+03
1024	8.00e+00	2.00e+03	4.51e+00	7.01e+03

Error in multiples of *eps*

Implementation Details

- Efficient storage and referencing of variables taking into account MATLAB's memory representation of arrays.

- Vectorization:

  Avoid loops where possible!

  Our implementation provides the possibility to specify the data functions for the right-hand side and the boundary conditions of the BVP in a vectorized format.

- Indexing — use of precomputed indices.

Comparisons

- `bvp4c` (MATLAB 6.0 standard routine)
  - Collocation at 3 Lobatto points
  - (Fixed) order 4
  - Provides no error estimate
  - Modifications for singular problems:
    Definition of right-hand side at $t = 0$
    Jacobian by finite differences
- COLNEW (Fortran 90 package)
  - Collocation at Gaussian points
  - Orders 2–14
  - Estimate: $h, h/2$ principle $\Longrightarrow$ finer grid
- `sbvp` (our package)
  - Coll. at equidistant/Gaussian points
  - Orders 2–16
  - Estimate: $2\times$ cheap auxiliary method

Comparisons (2)

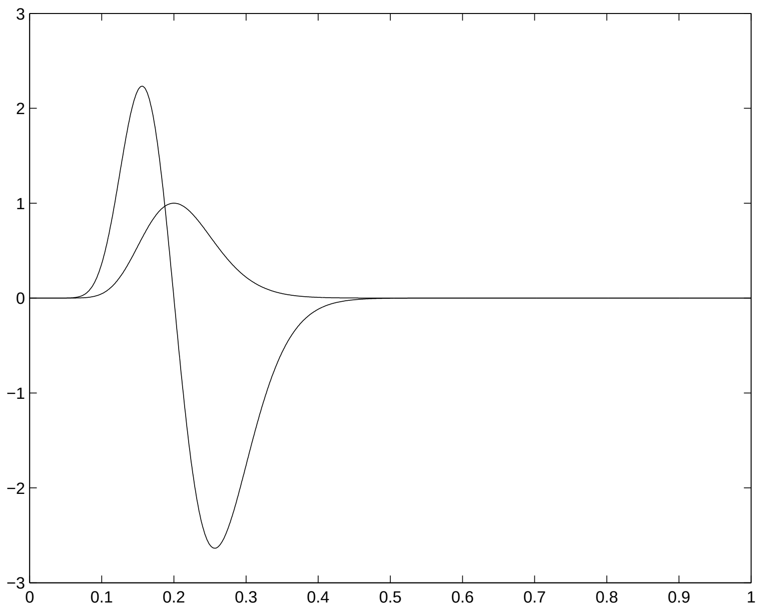
$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 1+\alpha^2 t^2 & 0 \end{pmatrix} z(t) + \\ + \begin{pmatrix} 0 \\ ct^{k-1}\mathrm{e}^{-\alpha t}(k^2 - 1 - \alpha t(1+2k)) \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ c\mathrm{e}^{-\alpha} \end{pmatrix},$$

where $\alpha = 80,\ k = 16$ and $c = \left(\frac{\alpha}{k}\right)^k \mathrm{e}^k$.

Exact solution:

$$z(t) = (ct^k \mathrm{e}^{-\alpha t}, ct^k \mathrm{e}^{-\alpha t}(k - \alpha t))^T.$$



Comparisons (3)

Hierher kommt die erste landscape-seite!

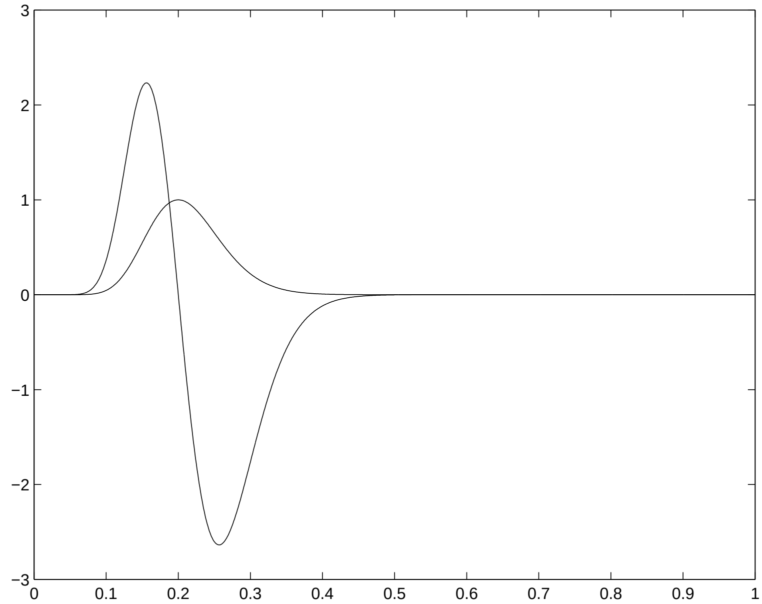
Comparisons (4)

2. landscape seite

Comparisons (5)

Meshes to reach the tolerances

$$\text{aTOL}=\text{rTOL}=10^{-5}$$



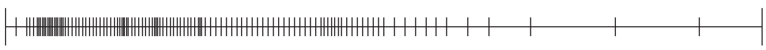


Figure 1: `bvp4c`, $N = 116$

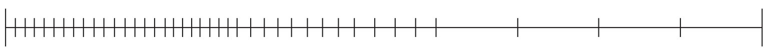


Figure 2: COLNEW-4, $N = 41$

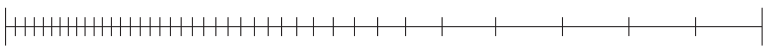


Figure 3: `sbvp4g`, $N = 40$

Comparisons (6)

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 2 & 6 \end{pmatrix} z(t) -$$

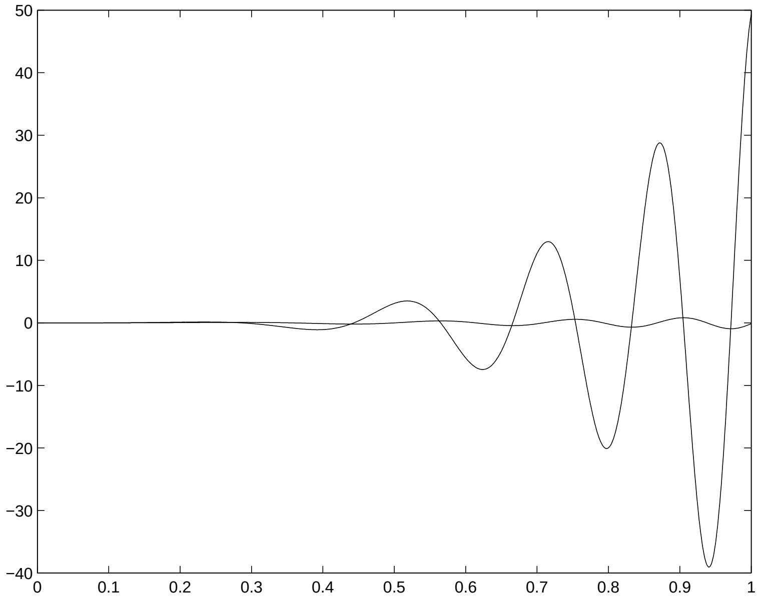
$$- \begin{pmatrix} 0 \\ 4k^4t^5\sin(k^2t^2) + 10t\sin(k^2t^2) \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ \sin(k^2) \end{pmatrix},$$

where $k = 5$.

Exact solution:

$$z(t) = (t^2\sin(k^2t^2), 2k^2t^4\cos(k^2t^2) + 2t^2\sin(k^2t^2))^T.$$



Comparisons (7)

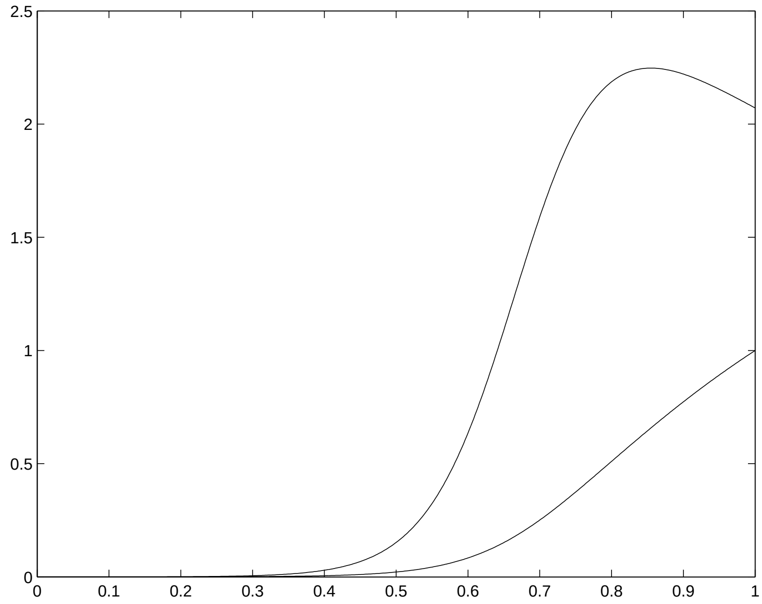
3. landscape seite

Comparisons (8)

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} z(t) +$$
$$+ \begin{pmatrix} 0 \\ t\phi^2 z_1(t)\exp\left(\frac{\gamma\beta(1-z_1(t))}{1+\beta(1-z_1(t))}\right) \end{pmatrix},$$
$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where $\phi = 0.6,\ \gamma = 40,\ \beta = 0.2.$

This problem has multiple solutions!



Comparisons (9)

4. landscape seite!

Conclusions & Future Work

- `sbvp` is competitive for **singular problems** with **smooth solutions**
- The results are most favorable for linear problems.
- We encountered problems when solving singular problems with unsmooth solutions.
- Regular problems with steep slopes:
  We are experimenting with a new mesh selection strategy.

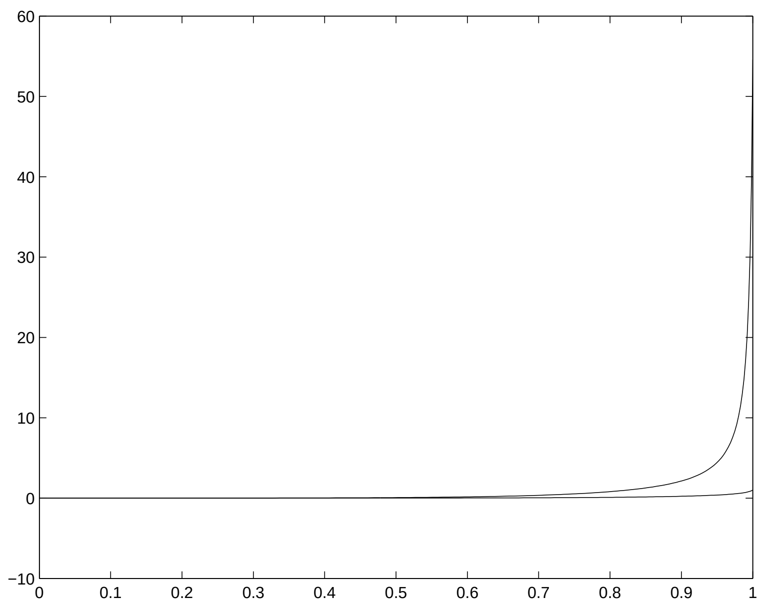
Conclusions & Future Work (2)

$$z'(t) = \begin{pmatrix} z_2(t) \\ n \sinh(n z_1(t)) \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where $n = 8$.

aTOL=rTOL=10^{-3}, $m = 6$.



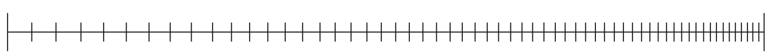


Figure 4: `sbvp`, $N = 61$, $h_{\max}/h_{\min} = 4.32$

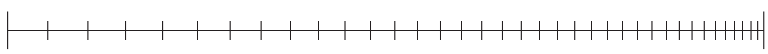


Figure 5: New strategy, $N = 38$, $h_{\max}/h_{\min} = 6.78$