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A note on two fixed point problems

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We dedicate this paper to Henryk Woźniakowski on the occasion of his 60th birthday

Abstract

We extend the applicability of the Exterior Ellipsoid Algorithm for approximating n-dimensional fixed points of directionally nonexpanding functions. Such functions model many practical problems that cannot be formulated in the smaller class of globally nonexpanding functions. The upper bound $2n^2 \ln(2/\varepsilon)$ on the number of function evaluations for finding ε-residual approximations to the fixed points remains the same for the larger class. We also present a modified version of a hybrid bisection-secant method for efficient approximation of univariate fixed point problems in combustion chemistry.

Keywords: Fixed point problems; Optimal algorithms; Nonlinear equations; Ellipsoid algorithm; Computational complexity

1. Introduction

An upper bound on the number of function evaluations needed to compute an ε-residual approximation $\mathbf{x}_\varepsilon$ to some fixed point of a function f, $\|f(\mathbf{x}_\varepsilon) - \mathbf{x}_\varepsilon\|_2 \leqslant \varepsilon$, for globally nonexpanding in the 2-nd norm function f, is $2n^2 \ln(1/\varepsilon)$ in n dimensions (see [3, Section 3]). This bound is realized by the Exterior Ellipsoid Algorithm (EEA). It is much better than the best known bounds $O((1/\varepsilon)^2)$ for the Krasnoselski–Mann type iterations [11], and is within a factor of n from the

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best possible bound $O(n\ln(1/\varepsilon))$, $\varepsilon \to 0$ [8,10] realized by the Centroid and Interior Ellipsoid algorithms (IEA).

At the conference in Bedlewo (Poland), co-organized in 2004 by Professor Woźniakowski, Dr. Vassin asked us if these bounds and algorithms could be extended to larger, more practical classes of functions that are only nonexpanding in the direction of fixed points. We stress that these larger classes contain functions that may be globally expanding, may be noncontinuous or may have unbounded derivatives. It turns out that the answer to Dr. Vassin's question is positive. We show with a simple proof, that the ellipsoid algorithms are applicable for the larger class and that the complexity bounds stay the same as for the globally nonexpanding functions. Several numerical tests of a new, numerically stable implementation of the EEA, as well as comparisons to simple iteration and Newton-type methods are presented in a separate paper [4].

We also introduce a univariate hyper-bisection/secant (HBS) method for approximating fixed points of certain combustion chemistry problems. That algorithm enjoys the average case number of iterations $O(\log\log(1/\varepsilon))$ for computing ε-absolute solutions. It is a modification of the bisection-secant method of Novak, Ritter and Woźniakowski that was proven by them to be optimal in the average case [12], with average number of function evaluations $O(\log\log(1/\varepsilon))$.

We stress that the ellipsoid algorithms are not applicable in the infinity-norm case, since the "cutting ball/plane" Lemma 3.1 that makes possible the construction of exterior/interior ellipsoids does not hold in that case. For the infinity norm case we developed a Bisection Envelope algorithm (BEFix) [14] and a Bisection Envelope Deep-Cut algorithm (BEDFix) [15] for approximating fixed points of two-dimensional nonexpanding functions. Those algorithms enjoy the minimal number of function evaluations $2\lceil\log_2(1/\varepsilon)\rceil + 1$. We also developed a (non-optimal) recursive fixed point algorithm (PFix) for approximating fixed points of n-dimensional nonexpanding functions with respect to the infinity norm (see [16,17]). We note that the minimal number of function evaluations needed for finding ε-residual solutions for expanding functions with the factor $\rho > 1$ is exponential $\Theta((\rho/\varepsilon)^{(n-1)})$, as $\varepsilon \to 0$ [7,6].

2. Classes of functions

Given the domain $B = \{\mathbf{x} \in \Re^n \mid \|\mathbf{x}\| \leqslant 1\}$, the n-dimensional unit ball, we consider the class of Lipschitz continuous functions:

$$\mathcal{B}_{\rho\leqslant 1} \equiv \{f : B \to B : \|f(\mathbf{x}) - f(\mathbf{y})\| \leqslant \rho\|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y} \in B\}, \tag{1}$$

where $n \geqslant 2$, $\|\cdot\| = \|\cdot\|_2$, and $0 < \rho \leqslant 1$. In the case when $0 < \rho < 1$, the class of functions is denoted by $\mathcal{B}_{\rho<1}$. The existence of fixed points α, $f(\alpha) = \alpha$, of functions f in $\mathcal{B}_{\rho\leqslant 1}$ is assured by the Brouwer's fixed point theorem [5].

The EEA algorithm computes an *absolute* ε*-approximation* $\mathbf{x}$ to α, $\|\mathbf{x} - \alpha\| \leqslant \varepsilon$ for every $f \in \mathcal{B}_{\rho<1}$, and computes a *residual* ε*-approximation* $\mathbf{x}_\varepsilon$, $\|f(\mathbf{x}_\varepsilon) - \mathbf{x}_\varepsilon\| \leqslant \varepsilon$ for every $f \in \mathcal{B}_{\rho\leqslant 1}$.

We extend the applicability of the EEA algorithm to directionally nonexpanding classes of functions considered by Vassin and Eremin in [26]. We indicate that the complexity bounds for the EEA algorithm do not change in this case. Those larger classes were investigated for problems defined by differential and integral equations originating in geophysics, atmospheric research, material science, and image deblurring [24,25,1,27,13]. These problems were effectively solved by Feyer-type iterative methods and/or some general optimization techniques; however,

no formal complexity bounds were derived. These classes are defined by

$$\mathcal{B}^{\alpha}_{\rho\leqslant 1} \equiv \{f : B \to B : \text{ the set of fixed points of } f,\ S(f) \neq \emptyset, \\ \text{and } \forall \mathbf{x} \in B, \text{ and } \forall \alpha \in S(f), \text{ we have } \|f(\mathbf{x}) - f(\alpha)\| \leqslant \rho \|\mathbf{x} - \alpha\|\}, \tag{2}$$

where $n \geqslant 2$ and $\rho \leqslant 1$. We note that the functions in $\mathcal{B}^{\alpha}_{\rho\leqslant 1}$ may be expanding globally, and therefore the class $\mathcal{B}_{\rho\leqslant 1}$ is a proper subclass of $\mathcal{B}^{\alpha}_{\rho\leqslant 1}$.

We finally introduce a univariate combustion chemistry fixed point problem defined in the class

$$G = \left\{ g : [a, b] \to [a, b] : g(t) = C_4 + \frac{C_5}{\left(\sqrt{\frac{C_1 t^2}{t - C_2} \cdot e^{-\frac{E_c}{Rt}} + C_3} + \sqrt{\frac{C_1 t^2}{t - C_2} \cdot e^{-\frac{E_c}{Rt}}} \right)^2} \right\}, \tag{3}$$

where the interval $[a, b]$, and the constants $C_1, \ldots, C_5$, R and E_c are explained in Section 4 .

We solve this problem in the equivalent zero finding formulation $f(x) = 0$, where $f(x) = x - g(x)$. We derive the HBS method that is a modification of the bisection/regula-falsi/secant (BRS) method which was proven almost optimal in the average case setting [12], with the complexity $O(\log\log(1/\varepsilon))$. To get ε-absolute approximations with $\varepsilon = 10^{-4}$ we need at most 6 function evaluations in the class G. Since the number of function evaluations in the HBS method is essentially bounded by the number of function evaluations in the BRS method, we conclude that the average case complexity of HBS is at most $O(\log\log(1/\varepsilon))$.

3. Constructive lemmas and cost bounds

The following "cutting ball/plane" lemma is the basis of the EEA algorithm for fixed points [19,21,23,20]. The proof of this lemma can be found in [21,20].

Lemma 3.1. *Let $f \in \mathcal{B}_{\rho<1}$. Suppose that $A \subseteq B$ contains the fixed point α. Then, for every $\mathbf{x} \in A$, $\alpha \in A \cap B(\mathbf{c}, \gamma)$, where $B(\mathbf{c}, \gamma) = \{x \in \Re^n : \|x - \mathbf{c}\| \leqslant \gamma\}$, $\mathbf{c} = \mathbf{x} + \frac{1}{1-\rho^2}(f(\mathbf{x}) - \mathbf{x})$ and $\gamma = \frac{\rho}{1-\rho^2}\|f(\mathbf{x}) - \mathbf{x}\|$.*

The following lemma and corollary exhibit upper bounds on the number of iterations of the EEA algorithm.

Lemma 3.2. *For any $\varepsilon \in (0, 1)$, and $f \in \mathcal{B}_{\rho\leqslant 1}$, the EEA algorithm requires at most $i = \left\lceil 2n(n+1)\ \ln\left(\frac{2+\varepsilon}{\varepsilon}\right)\right\rceil$ iterations to compute $\mathbf{x}_i \in \Re^n$ such that $\|f(\mathbf{x}_i) - \mathbf{x}_i\| \leqslant \varepsilon$, as $\varepsilon \to 0$.*

Proof. We give a sketch of the proof, since it follows the proof of Lemma 2.2 of Huang et al. [8].

The upper bound on the number of function evaluations of the EEA algorithm is obtained by replacing the volume reduction constant 0.861 from the IEA of Huang et al. [8], by the volume-reduction constant of the EEA algorithm given by $\exp(-1/(2(n+1))) < 1$ [9,20]. Following the

formula (2.3) of the proof in Huang et al. [8] we get

$$\frac{\varepsilon^n}{(2+\varepsilon)^n} \leqslant e^{-\frac{i}{2(n+1)}}. \tag{4}$$

The number of iterations that guarantees to obtain an ε-residual approximation $\mathbf{x}_i$ is the smallest i for which this inequality is violated. Therefore, we get

$$n \ln\left(\frac{2+\varepsilon}{\varepsilon}\right) \leqslant i \frac{1}{2(n+1)}, \tag{5}$$

that yields

$$i = \left\lceil 2n(n+1)\ln\left(\frac{2+\varepsilon}{\varepsilon}\right)\right\rceil,$$

and completes the proof.

We remark that the bound obtained in the above Lemma is better by a factor of n than the bound obtained in Tsay [23].

As a direct corollary from this lemma we get:

Corollary 3.3. *If $\rho < 1$, the EEA algorithm finds an ε-approximation $\mathbf{x}_i$ of the fixed point α in the absolute sense, $\|\mathbf{x}_i - \alpha\|_2 \leqslant \varepsilon$, within $i \cong 2n^2(\ln(2/\varepsilon) + \ln(1/(1-\rho))$ iterations.*

Proof. We observe that $\|x_i - \alpha\| \leqslant \frac{1}{1-\rho}\|x_i - f(x_i)\|$ and take $\varepsilon := \varepsilon(1-\rho)$ in Lemma 3.2.

Finally, we derive a constructive lemma for the larger class $B^{\alpha}_{\rho\leqslant 1}$. This lemma is similar in nature to Lemma 3.1, since after each function evaluation it enables us to locate the set of fixed points in the intersection of the previous set with a certain half space (in Lemma 3.1 it was the intersection of the previous set with a ball).

Lemma 3.4. *Let $f \in \mathcal{B}^{\alpha}_{\rho\leqslant 1}$ and $A \subset B$ be such that the set of fixed points $S(f) \subset A$. Then*:

$$\forall \mathbf{x} \in A, \quad S(f) \subset A \cap H_{\mathbf{x}}, \tag{6}$$

where the halfspace $H_{\mathbf{x}} = \{\mathbf{y} \in \Re^n : (\mathbf{y}-\mathbf{c})^T(f(\mathbf{x})-\mathbf{c}) \geqslant 0\}$, for $\mathbf{c} = (f(\mathbf{x})+\mathbf{x})/2$.

Proof. Suppose on the contrary that there exists $\alpha \in S(f)$ such that $(\alpha-\mathbf{c})^T(f(\mathbf{x})-\mathbf{c}) < 0$. Then, since $f(\mathbf{x}) - \mathbf{c} = \mathbf{c} - \mathbf{x}$, we get

$$\begin{aligned}
\|f(\mathbf{x}) - \alpha\|^2 &= (f(\mathbf{x}) - \mathbf{c} + \mathbf{c} - \alpha)^T(f(\mathbf{x}) - \mathbf{c} + \mathbf{c} - \alpha) \\
&= \|f(\mathbf{x}) - \mathbf{c}\|^2 + \|\mathbf{c} - \alpha\|^2 + 2(\mathbf{c}-\alpha)^T(f(\mathbf{x}) - \mathbf{c}) \\
&> \|f(\mathbf{x}) - \mathbf{c}\|^2 + \|\mathbf{c} - \alpha\|^2 \\
&> \|\mathbf{x} - \mathbf{c}\|^2 + \|\mathbf{c} - \alpha\|^2 - 2(\mathbf{c}-\alpha)^T(\mathbf{c} - \mathbf{x}) \\
&= \|\mathbf{x} - \mathbf{c} + \mathbf{c} - \alpha\|^2 = \|\mathbf{x} - \alpha\|^2,
\end{aligned} \tag{7}$$

which contradicts that $f \in \mathcal{B}^{\alpha}_{\rho\leqslant 1}$ and completes the proof. □

The above lemma implies that the EEA and IEA algorithms can also be applied to functions in $\mathcal{B}^{\alpha}_{\rho\leqslant 1}$ yielding the same complexity bounds as in the smaller classes $\mathcal{B}_{\rho\leqslant 1}$, since all of the arguments in the proof of Lemma 3.2 and Lemma 2.2 of Huang et al. [8] hold in the class $\mathcal{B}^{\alpha}_{\rho\leqslant 1}$. We formulate this conclusion in:

Lemma 3.5. *For any* $\varepsilon \in (0, 1)$, *and* $f \in \mathcal{B}^{\alpha}_{\rho\leqslant 1}$,

(i) *the EEA algorithm requires at most* $i = \left\lceil 2n(n+1)\cdot \ln\left(\frac{2+\varepsilon}{\varepsilon}\right)\right\rceil$ *iterations to compute* $\mathbf{x}_i \in \Re^n$ *such that* $\|f(\mathbf{x}_i) - \mathbf{x}_i\| \leqslant \varepsilon$, *as* $\varepsilon \to 0$, *and*

(ii) *the IEA algorithm requires at most* $k = \left\lceil 6.7n\ \ln\left(\frac{2+\varepsilon}{\varepsilon}\right)\right\rceil + 1$ *iterations to compute* $\mathbf{x}_k \in \Re^n$ *such that* $\|f(\mathbf{x}_k) - \mathbf{x}_k\| \leqslant \varepsilon$, *as* $\varepsilon \to 0$.

4. Combustion chemistry fixed point problem

In this section we focus on the design of a nearly optimal algorithm that is applied to univariate fixed point problems originating in modeling combustion of energetic materials. In particular, our algorithm is able to efficiently approximate fixed points of nonlinear equations modeling burning surface temperature of explosive materials. These fixed point calculations are utilized in large scale transient combustion simulations. They are repeated at every grid cell of a very large model and at every time step. This is why they have to be extremely fast and sufficiently accurate.

We derive an almost optimal (on the average) hyper-bisection/secant (HBS) modification of a hybrid bisection-regula falsi-secant (BRS) method [12] to solve a nonlinear fixed point problem that is derived from the Ward, Son, Brewster (WSB) combustion model [28–30]. This model implies [31] that the burning surface temperature T_s is a fixed point of the equation $T = G(T)$, where the function $G(.) = G_{P,T_0}(.)$ is uniquely defined by the initial gas phase pressure P and the initial solid temperature T_0, and is given by

$$G(T) = C_4 + \frac{C_5}{\left(\sqrt{\frac{C_1T^2}{T-C_2}\cdot e^{-\frac{E_c}{RT}} + C_3} + \sqrt{\frac{C_1T^2}{T-C_2}\cdot e^{-\frac{E_c}{RT}}}\right)^2},$$

where all constants C_i, E_c and R are positive. Those constants characterize the properties of materials and uniquely depend on the initial gas phase pressure P and the initial solid temperature T_0 [31]. We remark that the functions $G(\cdot)$ are in general expanding, and that in the univariate case we are able to find ε-absolute approximations to the fixed points of such functions with worst case complexity of $O(\log(1/\varepsilon))$ via the use of bisection-envelope algorithms [20]. In order to solve it even faster, we reformulate this fixed point problem as a zero finding problem: for function $f(T) = T - G(T)$ and a small positive number ε, we want to find an ε-approximation T_ε of the exact zero T_s of f, $f(T_s) = 0$, with respect to the root criterion $\frac{|T_\varepsilon - T_s|}{|T_{\max} - T_{\min}|} \leqslant \varepsilon$, where $[T_{\min}, T_{\max}]$ is the interval containing the solution T_s. It turns out [31] that we can set $T_{\min} = C_4$, and $T_{\max} = G(T_{s_{\max}})$ if $T_{\min} < T_{s_{\max}}$, or $T_{\max} = G(T_{\min})$ otherwise, where $T_{s_{\max}} = C_2 - \frac{E_c}{2R} + \sqrt{{C_2}^2 + \frac{{E_c}^2}{4R^2}}$. Since the function $f(\cdot)$ is continuous and has different signs at its endpoints, it follows that the exact zero T_s is in $[T_{\min}, T_{\max}]$.

Fig. 1 depicts a number of functions f with various T_0 and P.

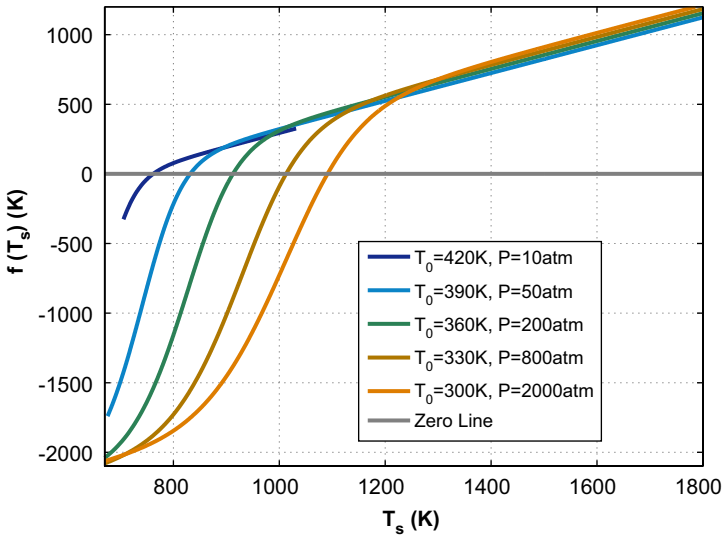

Fig. 1. Functions $f(T)$ with various T_0 and P.

4.1. Description of the algorithm

For the univariate zero finding problem, the solution can be efficiently obtained by using the BRS method that is almost optimal on the average [12].

4.1.1. The BRS method

We now outline the BRS method investigated in Novak et al. [12]. This method computes points $T_{s,i} \in [T_{\min}, T_{\max}]$, at which the function $f(\cdot)$ is evaluated, and a subinterval $[l_i, r_i]$ containing a zero of $f(\cdot)$. We always have $f(l_i) \leqslant 0 \leqslant f(r_i)$, $T_{s,i} \in \left[l_{i-1}, r_{i-1}\right]$ and $[l_i, r_i] \subset \left[l_{i-1}, r_{i-1}\right]$. Each function evaluation is preceded by the verification of the stopping rule. At the beginning and later after each bisection step, the method takes two steps of the regula falsi method, starting from the endpoints of the interval $\left[l_{i-1}, r_{i-1}\right]$. Then, the secant steps are performed until they are well defined, result in points in the current interval and reduce the length of the current interval by at least one half in every three steps. If any of these conditions is violated, a bisection step takes place. We utilize the absolute termination criterion given by

$$Stop_i = \begin{cases} 1 & \text{if } (r_i - l_i)/2 \leqslant \varepsilon \cdot (T_{\max} - T_{\min}) \quad \text{then } T_{s,i} = (l_i + r_i)/2, \\ 0 & \text{otherwise.} \end{cases}$$

After the termination ($Stop_i = 1$), we have $\frac{|T_{s,i} - T_s|}{|T_{\max} - T_{\min}|} \leqslant \varepsilon$, since the exact solution $T_s \in [l_i, r_i]$. We further define the points

$$Secant(u, w) = \begin{cases} u - \dfrac{f(u) \cdot (u - w)}{f(u) - f(w)} & \text{if } f(u) \neq f(w), \\ \text{undefined} & \text{otherwise,} \end{cases}$$

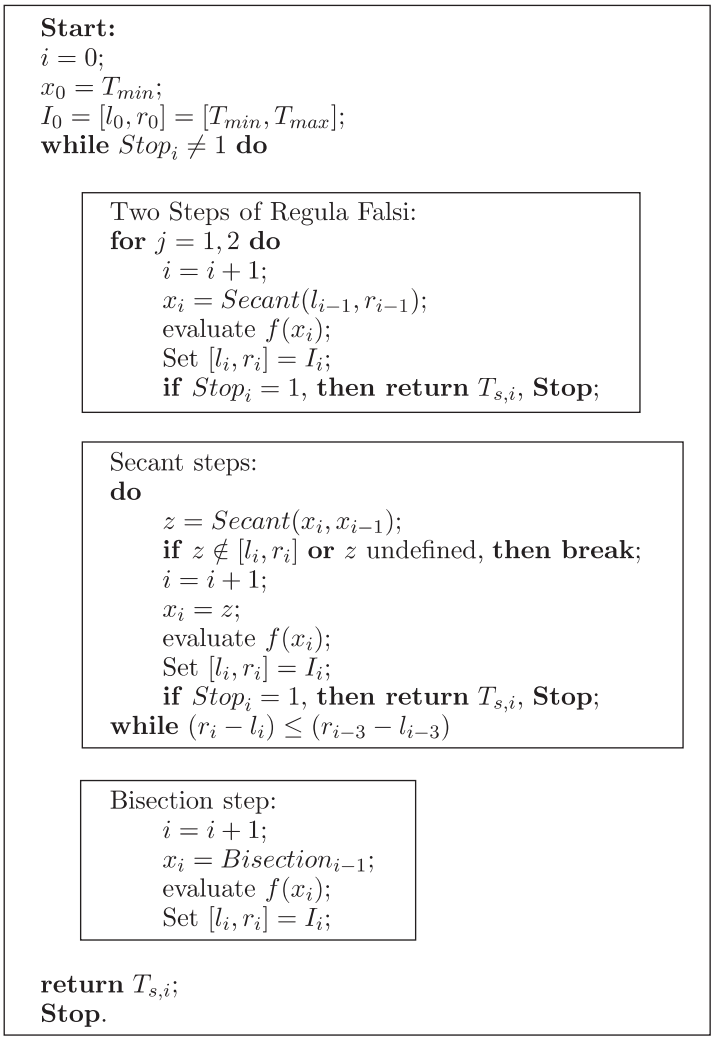

Fig. 2. Flowchart of the BRS method.

for the secant method with $u, w \in [T_{\min}, T_{\max}]$, and

$$Bisection_i = \frac{l_i + r_i}{2}$$

for the bisection method. In each step, a new interval I_i containing a zero of $f(T_s)$ is computed:

$$I_i = \begin{cases} [l_{i-1}, x_i] & \text{if } f(x_i) > 0, \\ [x_i, r_{i-1}] & \text{if } f(x_i) < 0, \\ [x_i, x_i] & \text{if } f(x_i) = 0. \end{cases}$$

The complete method is summarized in the flowchart in Fig. 2.

The BRS method is almost optimal on the average. The average number m_{aver} of function evaluations for finding an ε-approximation to the solution is bounded by

$$m_{\text{aver}} \leqslant \frac{1}{\log\left(\frac{1+\sqrt{5}}{2}\right)} \cdot \log\log\left(\frac{1}{\varepsilon}\right) + A,$$

where A is a constant [12].

For practical combustion simulations, the initial solid bulk temperature T_0 usually varies within the interval $TE = [280, 460]$ K and the gas phase pressure P within the interval $PR = [0, 3000]$ atm. To carry out the tests, we selected 60×50 evenly spaced grid nodes for the set of parameters $TE \times PR$. By choosing $\varepsilon = 10^{-4}$, the average number of iterations is 10.5, where the average is defined as the total number of iterations divided by the number of tested functions. We observed that for low P and high T_0 it took in the worst case 12–13 iterations to solve the problem. We derive the HBS, a modification to the BRS method, in order to lower the average and worst case numbers of iterations.

4.1.2. HBS method

To derive the HBS method, we first divide the parameter set $TE \times PR = [280, 460] \times [0, 3000]$ into three subdomains D_i, $i = 1, 2, 3$ by two lines $P = 4 \cdot (T_0 - 250)$ and $P = 15 \cdot (T_0 - 250)$,

$$D_i = \begin{cases} D_1 & \text{if } P \leqslant 4 \cdot (T_0 - 250), \\ D_2 & \text{if } 4 \cdot (T_0 - 250) < P \leqslant 15 \cdot (T_0 - 250), \\ D_3 & \text{if } P > 15 \cdot (T_0 - 250). \end{cases}$$

For each subdomain, we run two steps of hyper-bisection method defined as

$$Hyperbis_i = l_i + \xi_i \cdot (r_i - l_i),$$

where $\xi_i = \frac{T_{s,i} - l_i}{r_i - l_i} \in [0, 1]$. Extensive numerical experiments indicate that the solutions are distributed around the point $T_{\min} + \lambda \cdot (T_{\max} - T_{\min})$ in the sub-domain D_1, where $\lambda = 0.12$. We therefore utilize $\xi_1 = \lambda$ for the first step of hyper-bisection, and

$$\xi_2 = \begin{cases} \delta^2 & \text{if } f(Hyperbis_1) < 0, \\ 1 - \delta & \text{otherwise} \end{cases}$$

where $\delta = 0.2$. Those choices guarantee that in most cases the solution is in the interval $\left[Hyperbis_1, Hyperbis_2\right]$. The same strategy applies to subdomains D_2 and D_3, with $\lambda = 0.18$ for D_2 and $\lambda = 0.25$ for D_3. Parameter δ equals 0.2 for all subdomains. Ideally, the solution interval is reduced to 2–5% of its original length after two steps of the hyper-bisection. Thereafter, the BRS method is used to find the solution. When choosing the same set of test functions and $\varepsilon = 10^{-4}$, the average number of iterations of the HBS method is 5.7 (worst case 6) as compared to 10.5 (worst case 13) of the BRS method.

We remark that the secant method in the BRS algorithm could be replaced by the Newton's method in order to get asymptotically quadratic rate of convergence. This would however increase the cost of each iteration by a factor of at least two, since each step of Newton's method requires the computation of function value and the derivative, whenever the secant step only needs one function evaluation. As a result, the total computational cost would increase.

4.1.3. Conclusion

A hybrid bisection-secant method was developed for solving nonlinear equations derived from a combustion model. For the specific univariate zero finding problem, two more steps of a hyper-bisection method in addition to the original algorithm reduce the average number of iterations from 10.5 to 5.7. The worst case numbers of iterations are reduced from 13 to 6. This represents a significant improvement in the cost of carrying out large scale combustion simulations, since this zero finding problem has to be solved at every cell and every time step of billions of cells and millions of time steps.

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