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A MOVING ASYMPTOTES ALGORITHM USING NEW LOCAL CONVEX APPROXIMATION METHODS WITH EXPLICIT SOLUTIONS*

MOSTAFA BACHAR†, THIERRY ESTEBENET‡, AND ALLAL GUESSAB§

Abstract. In this paper we propose new local convex approximations for solving unconstrained non-linear optimization problems based on a moving asymptotes algorithm. This method incorporates second-order information for the moving asymptotes location. As a consequence, at each step of the iterative process, a strictly convex approximation subproblem is generated and solved. All subproblems have explicit global optima. This considerably reduces the computational cost of our optimization method and generates an iteration sequence. For this method, we prove convergence of the optimization algorithm under basic assumptions. In addition, we present an industrial problem to illustrate a practical application and a numerical test of our method.

Key words. geometric convergence, nonlinear programming, method of moving asymptotes, multivariate convex approximation

AMS subject classifications. 65K05, 65K10, 65L10, 90C30, 46N10

1. Motivation and theoretical justification. The so-called method of moving asymptotes (MMA) was introduced, without any global convergence analysis, by Svanberg [28] in 1987. This method can be seen as a generalization of the CONvex LINearization method (CONLIN); see [14], for instance. Later on, Svanberg [27] proposed a globally—but in reality slowly—convergent new method. Since then many different versions have been suggested. For more details on this topic see the references [3, 11, 12, 13, 18, 24, 25, 26, 30, 33, 34]. For reasons of simplicity, we consider the following unconstrained optimization problem: find $\boldsymbol{x}_* = (x_{*,1}, x_{*,2}, \ldots, x_{*,d})^\top \in \mathbb{R}^d$ such that

$$f(\boldsymbol{x}_*) = \min_{\boldsymbol{x}\in\mathbb{R}^d} f(\boldsymbol{x}), \tag{1.1}$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_d)^\top \in \mathbb{R}^d$ and f is a given non-linear, real-valued objective function, typically twice continuously differentiable. In order to introduce our extension of the original method more clearly, we will first present the most important facet of this approach. The MMA generates a sequence of convex and separable subproblems, which can be solved by any available algorithm taking into account their special structures. The idea behind MMA is the segmentation of the d-dimensional space into (d)-one-dimensional (1D) spaces.

Given the iteration points $\boldsymbol{x}^{(k)} = (x_1^{(k)}, x_2^{(k)}, \ldots, x_d^{(k)})^\top \in \mathbb{R}^d$ at the iteration k, then $L_j^{(k)}$ and $U_j^{(k)}$ are the lower and upper asymptotes that are adapted at each iteration step such that for $j = 1, \ldots, d$,

$$L_j^{(k)} < x_j < U_j^{(k)}.$$

During the MMA process, the objective function f is iteratively approximated at the k-th

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†Department of Mathematics, College of Sciences, King Saud University, Riyadh, Saudi Arabia (mbachar@ksu.edu.sa).

‡ALSTOM Ltd., Brown Boveri Strasse 10, CH-5401 Baden, Switzerland (thierry.estebenet@power.alstom.com).

§ Laboratoire de Mathématiques et de leurs Applications, UMR CNRS 4152, Université de Pau et des Pays de l'Adour, 64000 Pau, France (allal.guessab@univ-pau.fr).

iteration as follows:

$$\tilde{f}^{(k)}(\boldsymbol{x}) = r^{(k)} + \sum_{j=1}^{d} \frac{p_j^{(k)}}{U_j^{(k)} - x_j} + \frac{q_j^{(k)}}{x_j - L_j^{(k)}}.$$

The parameters $r^{(k)}$, $p_i^{(k)}$, and $q_i^{(k)}$ are adjusted such that a first-order approximation is satisfied, i.e.,

$$\tilde{f}^{(k)}(\boldsymbol{x}^{(k)}) = f(\boldsymbol{x}^{(k)}),$$
$$\nabla \tilde{f}^{(k)}(\boldsymbol{x}^{(k)}) = \nabla f(\boldsymbol{x}^{(k)}),$$

where $\nabla f(\boldsymbol{x})$ is the gradient of the objective function f at $\boldsymbol{x}$. The parameter $p_j^{(k)}$ is set to zero when $\frac{\partial \tilde{f}^{(k)}}{\partial x_j}(\boldsymbol{x}^{(k)}) < 0$, and $q_j^{(k)}$ is set to zero when $\frac{\partial \tilde{f}^{(k)}}{\partial x_j}(\boldsymbol{x}^{(k)}) > 0$ such that $\tilde{f}^{(k)}$ is a monotonically increasing or decreasing function of x_j. The coefficients $p_j^{(k)}$ and $q_j^{(k)}$ are then given respectively by

$$p_j^{(k)} = \left(U_j^{(k)} - x_j^{(k)}\right)^2 \max\left\{0, \frac{\partial \tilde{f}^{(k)}}{\partial x_j}(\boldsymbol{x}^{(k)})\right\},$$
$$q_j^{(k)} = \left(x_j^{(k)} - L_j^{(k)}\right)^2 \max\left\{0, -\frac{\partial \tilde{f}^{(k)}}{\partial x_j}(\boldsymbol{x}^{(k)})\right\}.$$

These parameters are strictly positive such that all approximating functions $\tilde{f}^{(k)}$ are strictly convex, and hence each subproblem has a single global optimum.

By this technique, the form of each approximated function is specified by the selected values of the parameters $L_j^{(k)}$ and $U_j^{(k)}$, which are chosen according to the specific MMA procedure. Several rules for selecting these values are discussed in detail in [4, 28]. Svanberg also shows how the parameters $L_j^{(k)}$ and $U_j^{(k)}$ can be used to control the general process. If the convergence process tends to oscillate, it may be stabilized by moving the asymptotes closer to the current iteration point, and if the convergence process is slow and monotonic, it may be relaxed by moving the asymptotes a limited distance away from their position in the current iteration. Several heuristic rules were also given for an adaptation process for automatic adjustment of these asymptotes at each iteration; see [27, 28]. The most important features of MMA can be summarized as follows.

- The MMA approximation is a first-order approximation at $\boldsymbol{x}^{(k)}$, i.e.,

$$\tilde{f}^{(k)}(\boldsymbol{x}^{(k)}) = f(\boldsymbol{x}^{(k)}),$$
$$\nabla \tilde{f}^{(k)}(\boldsymbol{x}^{(k)}) = \nabla f(\boldsymbol{x}^{(k)}).$$

- It is an explicit *rational*, strictly convex function for all $\boldsymbol{x}$ such that $L_j^{(k)} < x_j < U_j^{(k)}$ with poles (asymptotes in $L_j^{(k)}$ or in $U_j^{(k)}$), and it is monotonic (increasing if $\frac{\partial f}{\partial x_j}(\boldsymbol{x}^{(k)}) > 0$ and decreasing if $\frac{\partial f}{\partial x_j}(\boldsymbol{x}^{(k)}) < 0$).
- The MMA approximation is separable, which means that the approximation function $F : \mathbb{R}^d \to \mathbb{R}$ can be expressed as a sum of functions of the individual variables, i.e., there exist real functions $F_1, F_2, \cdots, F_d$ such that

$$F(\boldsymbol{x}) = F_1(x_1) + F_2(x_2) + \ldots + F_d(x_d).$$

Such a property is crucial in practice because the Hessian matrices of the approximations will be diagonal, and this allows us to address large-scale problems.

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- It is smooth, i.e., functions $\tilde{f}^{(k)}$ are twice continuously differentiable in the interval $L_j^{(k)} < x_j < U_j^{(k)}, j = 1, \dots, d$.
- At each outer iteration, given the current point $\boldsymbol{x}^{(k)}$, a subproblem is generated and solved, and its solution defines the next iteration $\boldsymbol{x}^{(k+1)}$, so only a single inner iteration is performed.

However, it should be mentioned that this method does not perform well in some cases and can even fail when the curvature of the approximation is not correctly assigned [23]. Indeed, it is important to realize that all convex approximations including MMA, which are based on first-order approximations, do not provide any information about the curvature. The second derivative information is contained in the Hessian matrix of the objective function $H[f]$, whose (i, j)-component is $\frac{\partial^2 f}{\partial x_i \partial x_j}(\boldsymbol{x})$. Updating the moving asymptotes remains a difficult problem. One possible approach is to use the diagonal second derivatives of the objective function in order to define the ideal values of these parameters in the MMA.

In fact, MMA was extended in order to include the first- and second-order derivatives of the objective function. For instance, a simple example of the MMA that uses a second-order approximation at iterate $\boldsymbol{x}^{(k)}$ was proposed by Fleury [14]:

$$\begin{aligned} \tilde{f}^{(k)}(\boldsymbol{x}) &= f(\boldsymbol{x}^{(k)}) \\ &\quad + \sum_{j=1}^{d} \left(\frac{1}{x_j^{(k)} - a_j^{(k)}} - \frac{1}{x_j - a_j^{(k)}} \right) \left(x_j^{(k)} - a_j^{(k)} \right)^2 \frac{\partial f}{\partial x_j}(\boldsymbol{x}^{(k)}), \end{aligned} \tag{1.2}$$

where, for each $j = 1, \dots, d$, the moving asymptote $a_j^{(k)}$ determined from the first and second derivatives is defined by

$$a_j^{(k)} = x_j^{(k)} + 2 \frac{\frac{\partial f}{\partial x_j}(\boldsymbol{x}^{(k)})}{\frac{\partial^2 f}{\partial x_j^2}(\boldsymbol{x}^{(k)})}.$$

Several versions have been suggested in the recent literature to obtain a practical implementation of MMA that takes full advantage of the second-order information, e.g., Bletzinger [2], Chickermane et al. [5], Smaoui et al. [23], and the papers cited therein provide additional reading on this topic. The limitations of the asymptote analysis method for first-order convex approximations are discussed by Smaoui et al. [23], where an approximation based on second-order information is compared with one based on only first-order. The second-order approximation is shown to achieve the best compromise between robustness and accuracy.

In contrast to the traditional approach, our method replaces the implicit problem (1.1) with a sequence of convex explicit subproblems having a simple algebraic form that can be solved *explicitly*. More precisely, in our method, an outer iteration starts from the current iterate $\boldsymbol{x}^{(k)}$ and ends up with a new iterate $\boldsymbol{x}^{(k+1)}$. At each inner iteration, within an *explicit* outer iteration, a convex subproblem is generated and solved. In this subproblem, the original objective function is replaced by *a linear* function plus *a rational function* which approximates the original functions around $\boldsymbol{x}^{(k)}$. The optimal solution of the subproblem becomes $\boldsymbol{x}^{(k+1)}$, and the outer iteration is completed. As in MMA, we will show that our approximation schemes share all the features listed above. In addition, our explicit iteration method is extremely simple to implement and is easy to use. Furthermore, MMA is very convenient to use in practice, but its theoretical convergence properties have not been studied exhaustively. This paper presents a detailed study of the convergence properties of the proposed method.

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The major motivation of this paper was to propose an approximation scheme which—as will be shown— meets all well-known properties of convexity and separability of the MMA. In particular, our proposed scheme provides the following major advantages:

1. An important aspect of our approximation scheme is that all its associated subproblems have *explicit* solutions.
2. It generates an iteration sequence that is bounded and converges to a stationary point of the objective function.
3. It converges geometrically.

The rest of the paper is organized as follows. For clarity of the discussion, the one-dimensional case is considered first. To this end, due to the separability of the approximations that we will consider later for the multivariate setting, we present our methodology for a single real variable in Section 2. In the following we show that the formulation extends to the multidimensional case. Indeed, Section 3 describes the extensions to more general settings than the univariate approach, where an explicit description of the proposed method will be derived and the corresponding algorithm will be presented. We also show that the proposed method has some favorable convergence properties. In order to avoid the evaluation of second derivatives, we will use a sequence of diagonal Hessian estimations, where only first- and zeroth-order information is accumulated during the previous iterations. We conclude Section 3 by giving a simple one-dimensional example which illustrates the performance of our method by showing that it has a wider convergence domain than the classical Newton's method. As an illustration, a realistic industrial inverse problem of multistage turbines using a through-flow code will be presented in Section 4. Finally, concluding remarks are offered in Section 5.

2. Univariate objective function. Since the simplicity of the one-dimensional case allows to detail all the necessary steps by very simple computations, let us first consider the general optimization problem (1.1) of a single real variable. To this end, we first list the necessary notation and terminology.

Let $d := 1$ and $\Omega \subset \mathbb{R}$ be an open subset and $f : \Omega \mapsto \mathbb{R}$ be a given twice differentiable function in Ω. Throughout, we assume that f' does not vanish at a given suitable initial point $x^{(0)} \in \Omega$, that is $f'(x^{(0)}) \neq 0$, since if this is not the case, we have nothing to solve. Starting from the initial design point $x^{(0)}$, the iterates $x^{(k)}$ are computed successively by solving subproblems of the form: find $x^{(k+1)}$ such that

$$f(x^{(k+1)}) = \min_{x \in \Omega} \tilde{f}^{(k)}(x),$$

where the approximating function $\tilde{f}^{(k)}$ of the objective function f at the k-th iteration has the following form

$$\begin{aligned} \tilde{f}^{(k)}(x) &= b^{(k)} + c^{(k)}(x - x^{(k)}) \\ &\quad + d^{(k)} \left(\frac{1}{2} \frac{\left(x^{(k)} - a^{(k)}\right)^3}{x - a^{(k)}} + \frac{1}{2} \left(x^{(k)} - a^{(k)}\right) \left(x - 2x^{(k)} + a^{(k)}\right) \right) \end{aligned} \tag{2.1}$$

with

$$a^{(k)} = \begin{cases} L^{(k)} & \text{if } f'(x^{(k)}) < 0 \text{ and } L^{(k)} < x^{(k)}, \\ U^{(k)} & \text{if } f'(x^{(k)}) > 0 \text{ and } U^{(k)} > x^{(k)}, \end{cases} \tag{2.2}$$

where the asymptotes $U^{(k)}$ and $L^{(k)}$ are adjusted heuristically as the optimization progresses or are guided by a proposed given function whose first and second derivative are evaluated at

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the current iteration point $x^{(k)}$. Also, the approximate parameters $b^{(k)}, c^{(k)}$, and $d^{(k)}$ will be determined for each iterations. To evaluate them, we use the objective function value, its first derivatives, as well as its second derivatives at $x^{(k)}$. The parameters $b^{(k)}, c^{(k)}$, and $d^{(k)}$ are determined in such a way that the following set of interpolation conditions are satisfied

$$\begin{aligned} \tilde{f}^{(k)}(x^{(k)}) &= f(x^{(k)}), \\ (\tilde{f}^{(k)})'(x^{(k)}) &= f'(x^{(k)}), \\ (\tilde{f}^{(k)})''(x^{(k)}) &= f''(x^{(k)}). \end{aligned} \tag{2.3}$$

Therefore, it is easy to verify that $b^{(k)}, c^{(k)}$, and $d^{(k)}$ are explicitly given by

$$\begin{aligned} b^{(k)} &= f(x^{(k)}), \\ c^{(k)} &= f'(x^{(k)}), \\ d^{(k)} &= f''(x^{(k)}). \end{aligned} \tag{2.4}$$

Throughout this section we will assume that

$$f''(x^{(k)}) > 0, \qquad \forall k \geq 0.$$

Let us now define the notion of feasibility for a sequence of asymptotes $\{a^{(k)}\} := \{a^{(k)}\}_k$, which we shall need in the following discussion.

DEFINITION 2.1. *A sequence of asymptotes $\{a^{(k)}\}$ is called feasible if for all $k \geq 0$, there exist two real numbers $L^{(k)}$ and $U^{(k)}$ satisfying the following condition:*

$$a^{(k)} = \begin{cases} L^{(k)} & \text{if } f'\left(x^{(k)}\right) < 0 \text{ and } L^{(k)} < x^{(k)} + 2\frac{f'\left(x^{(k)}\right)}{f''\left(x^{(k)}\right)}, \\ U^{(k)} & \text{if } f'\left(x^{(k)}\right) > 0 \text{ and } U^{(k)} > x^{(k)} + 2\frac{f'\left(x^{(k)}\right)}{f''\left(x^{(k)}\right)}. \end{cases}$$

It is clear from the above definition that every feasible sequence of asymptotes $\{a^{(k)}\}$ automatically satisfies all the constraints of type (2.2).

The following proposition, which is easily obtained by a simple algebraic manipulation, shows that the difference between the asymptotes and the current iterate $x^{(k)}$ can be estimated from below as in (2.5).

PROPOSITION 2.2. *Let $\{a^{(k)}\}$ be a sequence of asymptotes and let the assumptions (2.2) be valid. Then $\{a^{(k)}\}$ is feasible if and only if*

$$\frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})} < \left|x^{(k)} - a^{(k)}\right|. \tag{2.5}$$

It is interesting to note that our approximation scheme can be seen as an extension of Fleury's method [10]. Indeed, we have the following remark.

REMARK 2.3. Considering the approximations $\tilde{f}^{(k)}$ given in (2.1), if we write

$$\tilde{a}^{(k)} = x^{(k)} + \frac{2f'(x^{(k)})}{f''(x^{(k)})}$$

using the values of the parameters given in (2.4), the approximating functions $\tilde{f}^{(k)}$ can also be rewritten as

$$\begin{aligned} \tilde{f}^{(k)}(x) = f(x^{(k)}) &+ \frac{f''(x^{(k)})}{2}\left(\tilde{a}^{(k)} - a^{(k)}\right)\left(x - x^{(k)}\right) \\ &+ \frac{f''(x^{(k)})}{2}\left(x^{(k)} - a^{(k)}\right)^3 r^{(k)}(x), \end{aligned} \tag{2.6}$$

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with

$$r^{(k)}(x) = \left(\frac{1}{x - a^{(k)}} - \frac{1}{x^{(k)} - a^{(k)}} \right).$$

If we choose $\tilde{a}^{(k)} = a^{(k)}$, then the approximating functions become

$$\tilde{f}^{(k)}(x) = f(x^{(k)}) + \left(\frac{1}{x^{(k)} - a^{(k)}} - \frac{1}{x - a^{(k)}} \right) \left(x^{(k)} - a^{(k)} \right)^2 f'(x^{(k)}).$$

This is exactly the one-dimensional version of the approximation functions of Fleury given in equation (1.2). Hence, our approximation can be seen as a natural extension of Fleury's method [10].

The following lemma summarizes the basic properties of feasible sequences of asymptotes. In what follows, we denote by sign$(\cdot)$ the usual sign function.

LEMMA 2.4. *If $\{a^{(k)}\}$ is a feasible sequence of asymptotes, then for all k the following statements are true:*

i) $\frac{\text{sign}(f'(x^{(k)}))}{x^{(k)} - a^{(k)}} = -\frac{1}{|x^{(k)} - a^{(k)}|}$.

ii) $\frac{x^{(k)} - a^{(k)} + \frac{2f'(x^{(k)})}{f''(x^{(k)})}}{x^{(k)} - a^{(k)}} = \frac{|x^{(k)} - a^{(k)}| - \frac{2|f'(x^{(k)})|}{f''(x^{(k)})}}{|x^{(k)} - a^{(k)}|}$.

iii) At each iteration, the first derivative of the approximating function $\tilde{f}^{(k)}$ is given by

$$(\tilde{f}^{(k)})'(x) = \frac{f''(x^{(k)})}{2} \left(x^{(k)} - a^{(k)} \right) \left(e[f](x^{(k)}) - \left(\frac{x^{(k)} - a^{(k)}}{x - a^{(k)}} \right)^2 \right) \tag{2.7}$$

with

$$e[f](x^{(k)}) := \frac{|x^{(k)} - a^{(k)}| - \frac{2|f'(x^{(k)})|}{f''(x^{(k)})}}{|x^{(k)} - a^{(k)}|}.$$

Proof. The proof of $i)$ is straightforward since it is an immediate consequence of the fact that the sequence of asymptotes $\{a^{(k)}\}$ is feasible. We will only give a sketch of the proof of parts $ii)$ and $iii)$. By $i)$ and the obvious fact that

$$f'(x^{(k)}) = \text{sign}\left(f'(x^{(k)}) \right) \left| f'(x^{(k)}) \right|,$$

we have

$$\begin{aligned} \frac{x^{(k)} - a^{(k)} + \frac{2f'(x^{(k)})}{f''(x^{(k)})}}{x^{(k)} - a^{(k)}} &= 1 + \frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})} \frac{\text{sign}\left(f'(x^{(k)})\right)}{x^{(k)} - a^{(k)}} \\ &= 1 - \frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})} \frac{1}{\left|x^{(k)} - a^{(k)}\right|} \\ &= \frac{\left|x^{(k)} - a^{(k)}\right| - \frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})}}{\left|x^{(k)} - a^{(k)}\right|}. \end{aligned}$$

Finally, part $iii)$ is a consequence of part $ii)$ and the expression of $\tilde{f}^{(k)}$ given in (2.6). ∎

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By defining the suitable index set

$$\mathcal{I}^{(k)} = \begin{cases} \left]L^{(k)}, +\infty\right[& \text{if } f'\left(x^{(k)}\right) < 0, \\ \left]-\infty, U^{(k)}\right[& \text{if } f'\left(x^{(k)}\right) > 0, \end{cases}$$

we now are able to define our iterative sequence $\left\{x^{(k)}\right\}$. We still assume that f is a twice differentiable function in Ω satisfying $f''(x^{(k)}) > 0, \ \forall k \geq 0$.

THEOREM 2.5. *Using the above notation, let $\Omega \subset \mathbb{R}$ be an open subset of the real line, $x_0 \in \Omega$, and $x^{(k)}$ be the initial and the current point of the sequence $\left\{x^{(k)}\right\}$. Let the choice of the sequence of asymptotes $\left\{a^{(k)}\right\}$ be feasible. Then, for each $k \geq 0$, the approximated function $\tilde{f}^{(k)}$ defined by (2.1) is a strictly convex function in $\mathcal{I}^{(k)}$. Furthermore, for each $k \geq 0$, the function $\tilde{f}^{(k)}$ attains its minimum at*

$$x^{(k+1)} = a^{(k)} - \operatorname{sign}\left(f'(x^{(k)}\right)\sqrt{g^{(k)}}, \tag{2.8}$$

where

$$g^{(k)} := \frac{\left|x^{(k)} - a^{(k)}\right|^3}{\left|x^{(k)} - a^{(k)}\right| - \frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})}}.$$

Proof. An important characteristic of our approximate problem obtained via the approximation function $\tilde{f}^{(k)}$ is its strict convexity in $\mathcal{I}^{(k)}$. To prove strict convexity, we have to show that $(\tilde{f}^{(k)})''$ is non-negative in $\mathcal{I}^{(k)}$. Indeed, by a simple calculation of the second derivatives of $\tilde{f}^{(k)}$, we have

$$\left(\tilde{f}^{(k)}\right)''(x) = f''(x^{(k)})\left(\frac{x^{(k)} - a^{(k)}}{x - a^{(k)}}\right)^3.$$

Hence, to prove convexity of $\tilde{f}^{(k)}$, we have to show that

$$f''(x^{(k)})\left(\frac{x^{(k)} - a^{(k)}}{x - a^{(k)}}\right)^3 > 0, \qquad \forall x \in \mathcal{I}^{(k)}.$$

But $f''(x^{(k)}) > 0$ and so, according to the definition of the set $\mathcal{I}^{(k)}$, it follows that $x^{(k)} - a^{(k)}$ and $x - a^{(k)}$ have the same sign in the interval $\mathcal{I}^{(k)}$. Hence, we immediately obtain strict convexity of $\tilde{f}^{(k)}$ on $\mathcal{I}^{(k)}$. Furthermore, according to (2.7), if $\tilde{f}^{(k)}$ attains its minimum at $x_*^{(k)}$, then it is easy to see that $x_*^{(k)}$ is a solution of the equation

$$\left(\frac{x^{(k)} - a^{(k)}}{x - a^{(k)}}\right)^2 = \frac{\left|x^{(k)} - a^{(k)}\right| - \frac{2\left|f'(x^{(k)})\right|}{f''(x^{(k)})}}{\left|x^{(k)} - a^{(k)}\right|}. \tag{2.9}$$

Note that Proposition 2.2 ensures that the numerator of the term on the right-hand side is strictly positive. Now by taking the square root and using a simple transformation, we see that the unique solution $x_*^{(k)}$ belonging to $\mathcal{I}^{(k)}$ is given by (2.8). This completes the proof of the theorem. □

REMARK 2.6. At this point, we should remark that the notion of feasibility for a sequence of moving asymptotes, as defined in Definition 2.1, plays an important role for the existence of the *explicit* minimum given by (2.8) of the approximate function $\tilde{f}^{(k)}$ related to

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each subproblem belonging to $\mathcal{I}^{(k)}$. More precisely, it guarantees the positivity of the numerator of the fraction on the right-hand side of (2.9) and, hence, ensures the existence of a single global optimum for the approximate function at each iteration.

We now give a short discussion about an extension of the above approach. Our study in this section has been in a framework that at each iteration, the second derivative needs to be evaluated exactly. We will now focus our analysis on examining what happens when the second derivative of the objective function f may not be known or is expensive to evaluate. Thus, in order to reduce the computational effort, we suggest to approximate at each iteration the second derivative $f''(x^{(k)})$ by some positive real value $s^{(k)}$. In this situation, we shall propose the following procedure for selecting moving asymptotes:

$$\hat{a}^{(k)} = \begin{cases} L^{(k)} & \text{if } f'\left(x^{(k)}\right) < 0 \text{ and } L^{(k)} < x^{(k)} + 2\frac{f'\left(x^{(k)}\right)}{s^{(k)}}, \\ U^{(k)} & \text{if } f'\left(x^{(k)}\right) > 0 \text{ and } U^{(k)} > x^{(k)} + 2\frac{f'\left(x^{(k)}\right)}{s^{(k)}}. \end{cases} \tag{2.10}$$

It is clear that all the previous results easily carry over to the case when in the interpolation conditions (2.3), the second derivative $f''(x^{(k)})$ is replaced by an approximate (strictly) positive value $s^{(k)}$ according to the constraints (2.10). Indeed, the statements of Theorem 2.5 apply with straightforward changes.

In Section 3 for the multivariate case, we will discuss a strategy to determine at each iteration a reasonably good numerical approximation to the second derivative. We will also establish a multivariate version of Theorem 2.5 and show in this setting a general convergence result.

3. The multivariate setting. To develop our methods for the multivariate case, we need to replace the approximating functions (2.1) of the univariate objective function by suitable strictly convex multivariate approximating functions. The practical implementation of this method is considerably more complex than in the univariate case due to the fact that, at each iteration, the approximating function in the multivariate setting generates a sequence of diagonal Hessian estimates.

In this section, as well as in the case of univariate objective approximating function presented in Section 2, the function value $f(\boldsymbol{x}^{(k)})$, the first-order derivatives $\frac{\partial f(\boldsymbol{x}^{(k)})}{\partial x_j}$, for $j = 1 \ldots d$, as well as the second-order information and the moving asymptotes at the design point $\boldsymbol{x}^{(k)}$ are used to build up our approximation. To reduce the computational cost, the Hessian of the objective function at each iteration will be replaced by a sequence of diagonal Hessian estimates. These approximate matrices use only zeroth- and first-order information accumulated during the previous iterations. However, in view of practical difficulties of evaluating the second-order derivatives, a fitting algorithmic scheme is proposed in order to adjust the curvature of the approximation.

The purpose of the first part of this section is to give a complete discussion on the theoretical aspects concerning the multivariate setting of the convergence result established in Theorem 3.4 and to expose the computational difficulties that may be incurred. We will first describe the setup and notation for our approach. Below, we comment on the relationships between the new method and several of the most closely related ideas. Our approximation scheme leaves, as in the one-dimensional case, all well-known properties of convexity and separability of the MMA unchanged with the following major advantages:

1. All our subproblems have *explicit* solutions.
2. It generates an iteration sequence that is bounded and converges to a local solution.
3. It converges geometrically.

To simplify the notation, for every $j = 1, \ldots, d$, we use $f_{,j}$ to denote the first-order partial derivative of f with respect to each variable x_j. We also use the notation $f_{,,ij}$ for the second-order partial derivatives with respect to x_i first and then x_j. For any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, we will denote the standard inner product of $\boldsymbol{x}$ and $\boldsymbol{y}$ by $\langle \boldsymbol{x}, \boldsymbol{y} \rangle$ and $\|\boldsymbol{x}\| := \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$ the Euclidean vector norm of $\boldsymbol{x} \in \mathbb{R}^d$.

3.1. The convex approximation in $\boldsymbol{\Omega} \subset \mathbb{R}^d$. To build up the approximate optimization subproblems $P[k]$, taking into account the approximate optimization problem as a solution strategy of the optimization problem (1.1), we will seek to construct a successive sequence of subproblems $P[k], k \in \mathbb{N}$, at successive iteration points $\boldsymbol{x}^{(k)}$. That is, at each iteration k, we shall seek a suitable explicit rational approximating function $\tilde{f}^{(k)}$, strictly convex and relatively easy to implement. The solution of the subproblems $P[k]$ is denoted by $\boldsymbol{x}_*^{(k)}$, and will be obtained explicitly. The optimum $\boldsymbol{x}_*^{(k)}$ of the subproblems $P[k]$ will be considered as the starting point $\boldsymbol{x}^{(k+1)} := \boldsymbol{x}_*^{(k)}$ for the next subsequent approximate subproblems $P[k+1]$.

Therefore, for a given suitable initial approximation $\boldsymbol{x}^{(0)} \in \Omega$, the approximate optimization subproblems $P[k], k \in \mathbb{N}$, of the successive iteration points $\boldsymbol{x}^{(k)} \in \mathbb{R}^d$ can be written as: find $\boldsymbol{x}_*^{(k)}$ such that

$$\tilde{f}^{(k)}(\boldsymbol{x}_*^{(k)}) := \min_{\boldsymbol{x} \in \Omega} \tilde{f}^{(k)}(\boldsymbol{x}),$$

where the approximating function is defined by

$$\begin{aligned} \tilde{f}^{(k)}(\boldsymbol{x}) = \sum_{j=1}^{d} &\left(\frac{\left(\alpha_-^{(k)}\right)_j}{x_j - L_j^{(k)}} + \frac{\left(\alpha_+^{(k)}\right)_j}{U_j^{(k)} - x_j} \right) \\ &+ \left\langle \boldsymbol{\beta}_-^{(k)}, \boldsymbol{x} - \boldsymbol{L}^{(k)} \right\rangle + \left\langle \boldsymbol{\beta}_+^{(k)}, \boldsymbol{U}^{(k)} - \boldsymbol{x} \right\rangle + \gamma^{(k)}, \end{aligned} \tag{3.1}$$

and the coefficients $\boldsymbol{\beta}_-^{(k)}, \boldsymbol{\beta}_+^{(k)}, \boldsymbol{L}^{(k)}, \boldsymbol{U}^{(k)}$ are given by

$$\begin{aligned} \boldsymbol{\beta}_-^{(k)} &= \left(\left(\beta_-^{(k)}\right)_1, \ldots, \left(\beta_-^{(k)}\right)_d \right)^T, \\ \boldsymbol{\beta}_+^{(k)} &= \left(\left(\beta_+^{(k)}\right)_1, \ldots, \left(\beta_+^{(k)}\right)_d \right)^T, \\ \boldsymbol{L}^{(k)} &= \left(L_1^{(k)}, \ldots, L_d^{(k)} \right)^T, \\ \boldsymbol{U}^{(k)} &= \left(U_1^{(k)}, \ldots, U_d^{(k)} \right)^T, \end{aligned}$$

and $\gamma^{(k)} \in \mathbb{R}$. They represent the unknown parameters that need to be computed based on the available information. In order to ensure that the functions $\tilde{f}^{(k)}$ have suitable properties discussed earlier, we will assume that the following conditions (3.2) are satisfied for all k:

$$\begin{matrix} \left(\alpha_-^{(k)}\right)_j = \left(\beta_-^{(k)}\right)_j = 0 & \text{if } f_{,j}(\boldsymbol{x}^{(k)}) > 0, \\ \left(\alpha_+^{(k)}\right)_j = \left(\beta_+^{(k)}\right)_j = 0 & \text{if } f_{,j}(\boldsymbol{x}^{(k)}) < 0, \end{matrix} \qquad \text{for } j = 1, \ldots, d. \tag{3.2}$$

Our approximation can be viewed as a generalization of the univariate approximation to the multivariate case since the approximation functions $\tilde{f}^{(k)}$ are of the form of a linear function

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plus a rational function. It can easily be checked that the first- and second-order derivatives of $\tilde{f}^{(k)}$ have the following form

$$\tilde{f}^{(k)}_{,j}(\boldsymbol{x}) = \frac{-\left(\alpha_-^{(k)}\right)_j}{\left(x_j - L_j^{(k)}\right)^2} + \frac{\left(\alpha_+^{(k)}\right)_j}{\left(U_j^{(k)} - x_j\right)^2} + \left(\beta_-^{(k)}\right)_j - \left(\beta_+^{(k)}\right)_j, \quad j = 1,\dots,d, \tag{3.3}$$

$$\tilde{f}^{(k)}_{,,jj}(\boldsymbol{x}) = \frac{2\left(\alpha_-^{(k)}\right)_j}{\left(x_j - L_j^{(k)}\right)^3} + \frac{2\left(\alpha_+^{(k)}\right)_j}{\left(U_j^{(k)} - x_j\right)^3}, \qquad j = 1,\dots,d. \tag{3.4}$$

Now, making use of (3.2), these observations imply that if $f_{,j}(\boldsymbol{x}^{(k)}) > 0$, then

$$\tilde{f}^{(k)}_{,,jj}(\boldsymbol{x}) = \frac{2\left(\alpha_+^{(k)}\right)_j}{(U_j^{(k)} - x_j)^3}, \tag{3.5}$$

and if $f_{,j}(\boldsymbol{x}^{(k)}) < 0$, then

$$\tilde{f}^{(k)}_{,,jj}(\boldsymbol{x}) = \frac{2\left(\alpha_-^{(k)}\right)_j}{(x_j - L_j^{(k)})^3}. \tag{3.6}$$

Since the approximations $\tilde{f}^{(k)}$ are separable functions, all the mixed second derivatives of f are identically zero. Therefore, if $i \neq j$, we have

$$\tilde{f}^{(k)}_{,,ij}(\boldsymbol{x}) = 0, \qquad i, j = 1,\dots,d. \tag{3.7}$$

Also, the approximating functions $\tilde{f}^{(k)}$ need to be identically equal to the first-order approximations of the objective functions f at the current iteration point $\boldsymbol{x} = \boldsymbol{x}^{(k)}$, i.e.,

$$\begin{aligned} \tilde{f}^{(k)}\left(\boldsymbol{x}^{(k)}\right) &= f\left(\boldsymbol{x}^{(k)}\right), \\ \tilde{f}^{(k)}_{,j}\left(\boldsymbol{x}^{(k)}\right) &= f_{,j}\left(\boldsymbol{x}^{(k)}\right), \quad \forall j = 1,\dots,d. \end{aligned}$$

In addition to the above first-order approximations, the approximating function $\tilde{f}^{(k)}$ should include the information on the second-order derivatives f. Indeed, the proposed approximation will be improved if we impose that

$$\tilde{f}^{(k)}_{,,jj}\left(\boldsymbol{x}^{(k)}\right) = f_{,,jj}\left(\boldsymbol{x}^{(k)}\right), \ \forall j = 1,\dots,d. \tag{3.8}$$

Since the second derivatives of the original functions f may not be known or is expensive to evaluate, the above interpolation conditions (3.8) are not satisfied in general. However, it makes sense to use second-order derivative information to improve the convergence speed. The strategy of employing second-order information without excessive effort consists of approximating at each iteration the Hessian $H^{(k)}[f] := \left[f_{,,ij}\left(\boldsymbol{x}^{(k)}\right)\right]$ by a simple-structured and easily calculated matrix.

Our choice for approximating the derivatives is based on the spectral parameters as detailed in [16], where the Hessian of the function f is approximated by the diagonal matrix $S^{(k)}_{jj} I$ (i.e., $\eta^{(k)} I$ in [15, 16]), with I the d-by-d identity matrix, and the coefficients $S^{(k)}_{jj}$

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are simply chosen such that

$$S_{jj}^{(k)} := \frac{d^{(k)}}{\left\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\right\|^2} \approx f_{,,jj}\left(\boldsymbol{x}^{(k)}\right), \tag{3.9}$$

where

$$d^{(k)} := \langle \nabla f(\boldsymbol{x}^{(k)}) - \nabla f(\boldsymbol{x}^{(k-1)}), \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \rangle > 0. \tag{3.10}$$

The last conditions (3.10) ensure that the approximations $\tilde{f}^{(k)}$ are strictly convex for all iterates $\boldsymbol{x}^{(k)}$ since the parameters $S_{jj}^{(k)}$ are chosen as strictly positive.

Thus, if we use the three identities (3.5), (3.6), (3.7), and the above approximation conditions, we get after some manipulations that

$$\left(\alpha_-^{(k)}\right)_j = \begin{cases} \frac{1}{2} S_{jj}^{(k)} \left(x_j^{(k)} - L_j^{(k)}\right)^3 & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) < 0, \\ 0 & \text{otherwise}, \end{cases} \tag{3.11}$$

$$\left(\alpha_+^{(k)}\right)_j = \begin{cases} \frac{1}{2} S_{jj}^{(k)} \left(U_j^{(k)} - x_j^{(k)}\right)^3 & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) > 0, \\ 0 & \text{otherwise}, \end{cases} \tag{3.12}$$

$$\left(\beta_-^{(k)}\right)_j = \begin{cases} f_{,j}\left(\boldsymbol{x}^{(k)}\right) + \frac{\left(\alpha_-^{(k)}\right)_j}{\left(x_j^{(k)} - L_j^{(k)}\right)^2} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) < 0, \\ 0 & \text{otherwise}, \end{cases} \tag{3.13}$$

$$\left(\beta_+^{(k)}\right)_j = \begin{cases} f_{,j}\left(\boldsymbol{x}^{(k)}\right) - \frac{\left(\alpha_+^{(k)}\right)_j}{\left(U_j^{(k)} - x_j^{(k)}\right)^2} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) > 0, \\ 0 & \text{otherwise}, \end{cases} \tag{3.14}$$

and

$$\begin{aligned} \gamma^{(k)} = f\left(\boldsymbol{x}^{(k)}\right) &- \sum_{j=1}^{d} \left(\frac{\left(\alpha_-^{(k)}\right)_j}{x_j^{(k)} - L_j^{(k)}} + \frac{\left(\alpha_+^{(k)}\right)_j}{U_j^{(k)} - x_j^{(k)}} \right) \\ &- \left\langle \boldsymbol{\beta}_-^{(k)}, \boldsymbol{x}^{(k)} - \boldsymbol{L}^{(k)} \right\rangle - \left\langle \boldsymbol{\beta}_+^{(k)}, \boldsymbol{U}^{(k)} - \boldsymbol{x}^{(k)} \right\rangle. \end{aligned}$$

Our strategy will be to update the lower and upper moving asymptotes, $L_j^{(k)}$ and $U_j^{(k)}$, at each iteration based on second-order information by generalizing Definition 2.1 from Section 2. Since the approximation functions are separable, only the first-order derivatives and the approximate second-order diagonal Hessian terms are required in the process. Smaoui et al. [23] also use such a second-order strategy, but here $f_{,,jj}\left(\boldsymbol{x}^{(k)}\right)$ is replaced by the estimated value $S_{jj}^{(k)}$ given in (3.9) as follows:

$$\begin{aligned} A_j^{(k)} &= \begin{cases} L_j^{(k)} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) < 0 \text{ and } L_j^{(k)} < x_j^{(k)} + 2\frac{f_{,j}\left(\boldsymbol{x}^{(k)}\right)}{S_{jj}^{(k)}}, \\ U_j^{(k)} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) > 0 \text{ and } U_j^{(k)} > x_j^{(k)} + 2\frac{f_{,j}\left(\boldsymbol{x}^{(k)}\right)}{S_{jj}^{(k)}}, \end{cases} \\ \boldsymbol{A}^{(k)} &= (A_1^{(k)}, A_2^{(k)}, \ldots, A_d^{(k)})^\top. \end{aligned} \tag{3.15}$$

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Note that, as it was done in the univariate case, see Proposition 2.2, we have the following result.

PROPOSITION 3.1. *Let $\boldsymbol{A}^{(k)} = (A_1^{(k)}, A_2^{(k)}, \ldots, A_d^{(k)})^\top \in \mathbb{R}^d$ be the moving asymptotes with components given by (3.15). Then, for all $j = 1, \ldots, d$, and for all k, we have*

$$\frac{2|f_{,j}(\boldsymbol{x}^{(k)})|}{S_{jj}^{(k)}} < \left| x_j^{(k)} - A_j^{(k)} \right|.$$

To define our multivariate iterative scheme, we start from some given suitable initial approximation $\boldsymbol{x}^{(0)} \in \Omega$ and let $\{\boldsymbol{x}^{(k)}\} := \left\{\boldsymbol{x}^{(k)}\right\}_k$ be the iterative sequence defined by $\boldsymbol{x}^{(k+1)} = (x_1^{(k+1)}, \ldots, x_d^{(k+1)})^T$, for all $k \geq 0$ and $j = 1 \ldots, d$, with

$$x_j^{(k+1)} = A_j^{(k)} - \text{sign}\left(f_{,j}\left(\boldsymbol{x}^{(k)}\right)\right)\sqrt{g_j^{(k)}},\ (j = 1, \ldots, d), \tag{3.16}$$

where

$$g_j^{(k)} = \frac{\left|x_j^{(k)} - A_j^{(k)}\right|^3}{\left|x_j^{(k)} - A_j^{(k)}\right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k)}\right)\right|}{S_{jj}^{(k)}}} = \begin{cases} \dfrac{\left(\alpha_-^{(k)}\right)_j}{\left(\beta_-^{(k)}\right)_j} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) < 0, \\[2ex] \dfrac{\left(\alpha_+^{(k)}\right)_j}{-\left(\beta_+^{(k)}\right)_j} & \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) > 0. \end{cases} \tag{3.17}$$

It should be pointed out that the sequence $\left\{\boldsymbol{x}^{(k)}\right\}$ is well-defined for all k since the denominators of (3.16) never vanish, and it is straightforward to see that the values $g_j^{(k)}$ in (3.17) are positive real numbers.

It would be more precise to use the set notation and write: $\mathcal{I}^{(k)} = \mathcal{I}_1^{(k)} \times \mathcal{I}_2^{(k)} \times \cdots \times \mathcal{I}_d^{(k)}$, with

$$\mathcal{I}_j^{(k)} = \begin{cases} \left]L_j^{(k)}, +\infty\right[& \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) < 0, \\ \left]-\infty, U_j^{(k)}\right[& \text{if } f_{,j}\left(\boldsymbol{x}^{(k)}\right) > 0, \end{cases} \qquad j = 1, \ldots, d.$$

Now we are in a position to present one main result of this paper.

THEOREM 3.2. *Let Ω be a given open subset of $\mathbb{R}^d$ and $f : \Omega \to \mathbb{R}$ be a twice-differentiable objective function in Ω. We assume that the moving asymptotes $\boldsymbol{A}^{(k)} \in \mathbb{R}^d$ are defined by equations (3.15), where $S_{jj}^{(k)} > 0, k \geq 0, j = 1, \ldots, d$, and let $\left\{\boldsymbol{x}^{(k)}\right\}$ be the iterative sequence defined by (3.16). Then the objective function $\tilde{f}^{(k)}$ defined by equation (3.1) with the coefficients (3.11)–(3.14) is a first-order strictly convex approximation of f that satisfies*

$$f_{,,jj}^{(k)}\left(\boldsymbol{x}^{(k)}\right) = S_{jj}^{(k)}, \qquad j = 1, \ldots, d.$$

Furthermore, $f^{(k)}$ attains its minimum at $\boldsymbol{x}^{(k+1)}$.

Proof. By construction, the approximation $\tilde{f}^{(k)}$ is a first-order approximation of f at $\boldsymbol{x} = \boldsymbol{x}^{(k)}$ and satisfies

$$f_{,,jj}^{(k)}\left(\boldsymbol{x}^{(k)}\right) = S_{jj}^{(k)}, \qquad \forall j = 1, \ldots, d.$$

As $(\alpha_-^{(k)})_j$ (respectively $(\alpha_+^{(k)})_j$) has the same sign as $\boldsymbol{x}_j - L_j^{(k)}$ (respectively $U_j^{(k)} - \boldsymbol{x}_j$) in $\mathcal{I}^{(k)}$, we can easily deduce from (3.4) that the approximation is strictly convex in $\mathcal{I}^{(k)}$.

In addition, by using (3.3), we may verify that $\boldsymbol{x}^{(k+1)}$ given by (3.16) is the unique solution in $\mathcal{I}^{(k)}$ of the equations

$$f_{,j}^{(k)}(\boldsymbol{x}) = 0, \qquad \forall j = 1, \dots, d,$$

which completes the proof of the theorem. □

The sequence of subproblems generated by (3.16) is computed by Algorithm 3.3.

ALGORITHM 3.3. *Method of the moving asymptotes with spectral updating.*

Step 1. *Initialization*

Define $\boldsymbol{x}^{(0)}$
Set $k \leftarrow 0$

Step 2. *Stopping criterion*

If $\boldsymbol{x}^{(k)}$ satisfies the convergence conditions of the problem (1.1), then stop and take $\boldsymbol{x}^{(k)}$ as the solution.

Step 3. *Computation of the spectral parameters $S_{jj}^{(k)}$, the moving asymptotes $A_j^{(k)}$, and the intermediate parameter $g_j^{(k)}$:*

Compute
$d^{(k)} = \langle \nabla f(\boldsymbol{x}^{(k)}) - \nabla f(\boldsymbol{x}^{(k-1)}), \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \rangle$,
For $j = 0, 1, ..., d$

$$S_{jj}^{(k)} = \frac{d^{(k)}}{\left\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\right\|^2},$$

$$A_j^{(k)} = x_j^{(k)} + 2\alpha \frac{f_{,j}\left(\boldsymbol{x}^{(k)}\right)}{S_{jj}^{(k)}}, \ \alpha > 1,$$

$$g_j^{(k)} = \frac{\left|x_j^{(k)} - A_j^{(k)}\right|^3}{\left|x_j^{(k)} - A_j^{(k)}\right| - 2\frac{\left|f_{,j}\left(\boldsymbol{x}^{(k)}\right)\right|}{S_{jj}^{(k)}}}.$$

Step 4. *Computation of the solution of the subproblem*

$$x_j^{(k+1)} = A_j^{(k)} - \text{sign}\left(f_{,j}\left(\boldsymbol{x}^{(k)}\right)\right)\sqrt{g_j^{(k)}} \qquad \text{for } j = 0, 1, ..., d,$$

Set $k \leftarrow k+1$
Go to **Step 2.**

3.2. A multivariate convergence result. This subsection aims to show that the proposed method is convergent in the sense that the optimal iterative sequence $\left\{\boldsymbol{x}^{(k)}\right\}$ generated by Algorithm 3.3 converges geometrically to $\boldsymbol{x}_*$. That is, there exists a $\xi \in]0, 1[$ such that

$$\|\boldsymbol{x}^{(k)} - \boldsymbol{x}_*\| \leq \frac{\xi^k}{1-\xi}\|\boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)}\|.$$

To this end, the following assumptions are required. Let us suppose that there exist positive constants r, M, C, and $\xi < 1$ such that the following assumptions hold.

Assumption M1:

$$B_r := \{x \in \mathbb{R} : \|\boldsymbol{x} - \boldsymbol{x}^{(0)}\| \leq r\} \subset \Omega.$$

Assumption M2: We assume that the sequence of moving asymptotes $\{\boldsymbol{A}^{(k)}\}$ defined by (3.15) satisfies

$$\sup_{k \geq 0} \|\boldsymbol{x}^{(k)} - \boldsymbol{A}^{(k)}\| \leq C, \tag{3.18}$$

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and for all $j = 1, \ldots, d$,

$$\frac{2C\sqrt{d}}{MS_{jj}^{(k)}} \leq \left| x_j^{(k)} - A_j^{(k)} \right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k)}\right)\right|}{S_{jj}^{(k)}}. \tag{3.19}$$

Assumption M3: We require that for all $k > 0$ and for all $j \in \{1, \ldots, d\}$ with $x_j^{(k-1)} \neq x_j^{(k)}$,

$$\sup_{k>0} \sup_{x \in B} \left\| \nabla f_{,j}(\boldsymbol{x}) - \frac{f_{,j}(\boldsymbol{x}^{(k-1)})}{x_j^{(k-1)} - x_j^{(k)}} \boldsymbol{e}^{(j)} \right\| \leq \frac{\xi}{M}, \tag{3.20}$$

where $\boldsymbol{e}^{(j)}$ is the vector of $\mathbb{R}^d$ with the j-th component equal to 1 and all other components equal to 0.

Assumption M4: For all $j = 1, \ldots, d$, the initial iterate $\boldsymbol{x}^0$ satisfies

$$0 < |f_{,j}(\boldsymbol{x}^0)| \leq \frac{r}{M}(1 - \xi).$$

Let us briefly comment on these assumptions.

- First, in order to control the feasibility of the moving asymptotes, we need to find a (strictly) positive lower bound of

$$|x_j^{(k)} - A_j^{(k)}| - \frac{2|f_{,j}(\boldsymbol{x}^{(k)})|}{S_{jj}^{(k)}}, \tag{3.21}$$

  which needs to be large according to some predetermined tolerance; see Proposition 3.1. So when the inequalities (3.19) hold, then the sequence of the moving asymptotes $\left\{\boldsymbol{A}^{(k)}\right\}$ is automatically feasible. Also note that, when we evaluate the approximate function $\tilde{f}^{(k)}$ and if the difference between the asymptotes and the current iteration point is small enough, then imposing condition (3.19) avoids the possibility of (3.21) to become negative or close to zero. In Assumption M2, inequality (3.18) enforces the quite natural condition that at each iteration k, the distance between $\boldsymbol{x}^{(k)}$ and the asymptote $A^{(k)}$ is bounded above by some constant.
- Assumption M3 ensures that $\nabla f_{,j}(\boldsymbol{x})$ is sufficiently close to $\frac{f_{,j}(\boldsymbol{x}^{(k-1)})}{x_j^{(k-1)} - x_j^{(k)}} \boldsymbol{e}^{(j)}$.
- Assumption M4, as we will see, is only used to obtain uniqueness of the limit of the iteration sequence generated by Theorem 3.2. The convergence result is established without this assumption. It also requires that $|f_{,j}(\boldsymbol{x}^0)|$ to be small enough and that $f_{,j}(\boldsymbol{x}^0)$ is not equal to 0. This assumption will also play an important role when showing that ∇f has a unique zero in B_r.

Assumptions M2 and M3 will be used in conjunction with Assumption M4 to prove that the sequence of iteration points $\left\{\boldsymbol{x}^{(k)}\right\}$ defined by (3.16) has various nice properties and converges geometrically to the unique zero of ∇f in B_r. In addition, note that the constant C ensures that the distances between the current points $\boldsymbol{x}^{(k)}$ and the moving asymptotes are finite, and the constant M ensures that the process starts reasonably close to the solution.

We are now prepared to state and to show our main convergence result.

THEOREM 3.4. *Given Assumptions M1–M4, the sequence $\left\{\boldsymbol{x}^{(k)}\right\}$ defined in (3.16) is completely contained in the closed ball B_r and converges geometrically to the unique stationary point of f belonging to the ball B_r.*

Before we prove Theorem 3.4, we present some preparatory lemmas. The first key ingredient is the following simple observation.

LEMMA 3.5. *Let k be a fixed positive integer. Assume that there exists an index $j \in \{1, \ldots, d\}$ such that $f_{,j}(\boldsymbol{x}^{(k-1)}) \neq 0$. Then the j-th components of the two successive iterates $\boldsymbol{x}^{(k)}$ and $\boldsymbol{x}^{(k-1)}$ are distinct.*

Proof. Indeed, assume the contrary, that is $x_j^{(k)} = x_j^{(k-1)}$. Then from equation (3.16), we have

$$\begin{aligned}\left(x_j^{(k-1)} - A_j^{(k-1)}\right)^2 &= \left(x_j^{(k)} - A_j^{(k-1)}\right)^2 \\ &= g_j^{(k-1)} \\ &= \frac{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|^3}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)\right|}{S_{jj}^{(k-1)}}},\end{aligned}$$

or equivalently $f_{,j}\left(\boldsymbol{x}^{(k-1)}\right) = 0$, which leads to a contradiction and proves the lemma. ∎

REMARK 3.6. The previous lemma states that if the j-th partial derivative of f does not vanish at the iterate $\boldsymbol{x}^{(k-1)}$, then the required condition in Assumption M4 is satisfied.

We will also need to prove a useful lemma, which bounds the distance between two consecutive iterates $\boldsymbol{x}^{(k-1)}$ and $\boldsymbol{x}^{(k)}$.

LEMMA 3.7. *Let Assumptions M2–M4 be satisfied, and let the sequence $\left\{\boldsymbol{x}^{(k)}\right\}$ be defined as in equation (3.16). Then, the following inequalities hold for all positive integers k and $j = 1, \ldots, d$,*

$$\begin{aligned}\left|x_j^{(k)} - x_j^{(k-1)}\right| &\leq \frac{M}{\sqrt{d}}\left|f_{,j}(\boldsymbol{x}^{(k-1)})\right|, \\ \left\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\right\| &\leq M \max_{1\leq j\leq d}\left|f_{,j}(\boldsymbol{x}^{(k-1)})\right|.\end{aligned}$$

Proof. Let us fix an integer k such that $k > 0$. Then using (3.16), $x_j^{(k)} - x_j^{(k-1)}$ can be written in the form

$$\begin{aligned}x_j^{(k)} - x_j^{(k-1)} &= A_j^{(k-1)} - \text{sign}\left(f_{,j}(\boldsymbol{x}^{(k-1)})\right)\sqrt{g_j^{(k-1)}} - x^{(k-1)} \\ &= (x_j^{(k-1)} - A_j^{(k-1)})\,(-1 + \Delta)\,,\end{aligned} \tag{3.22}$$

where, in the last equality, we have denoted

$$\Delta = \frac{-\text{sign}(f_{,j}(\boldsymbol{x}^{(k-1)}))}{x_j^{(k-1)} - A_j^{(k-1)}}\sqrt{g_j^{(k-1)}}.$$

Now, as in one dimension, see Lemma 2.4, it is easy to verify that

$$\frac{\text{sign}(f_{,j}(\boldsymbol{x}^{(k-1)}))}{x_j^{(k-1)} - A_j^{(k-1)}} = -\frac{1}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|}\,.$$

Consequently Δ also can be expressed in fraction form

$$\Delta = \frac{\sqrt{g^{(k-1)}}}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|}\,.$$

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Since

$$g_j^{(k-1)} := \frac{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|^3}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)\right|}{S_{jj}^{(k-1)}}},$$

it follows from (3.22) that

$$\left|x_j^{(k)} - x_j^{(k-1)}\right| \leq \left|x_j^{(k-1)} - A_j^{(k-1)}\right| \left(\sqrt{\tilde{g}^{(k-1)}} - 1\right) \tag{3.23}$$

with

$$\tilde{g}^{(k-1)} := \frac{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)\right|}{S_{jj}^{(k-1)}}}.$$

Taking into account that $\tilde{g}^{(k-1)} > 1$ and using the square root property, we get

$$\sqrt{\tilde{g}^{(k-1)}} < \tilde{g}^{(k-1)}.$$

Therefore, by (3.23), we conclude that

$$\left|x_j^{(k)} - x_j^{(k-1)}\right| \leq \frac{\left|x_j^{(k-1)} - A_j^{(k-1)}\right|}{\left|x_j^{(k-1)} - A_j^{(k-1)}\right| - \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)\right|}{S_{jj}^{(k-1)}}} \frac{2\left|f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)\right|}{S_{jj}^{(k-1)}}.$$

We now obtain the desired conclusion by using Assumption M2. The second inequality in Lemma 3.7 is an immediate consequence of the definition of the Euclidean norm.

$\square$

Now, we are ready to prove Theorem 3.4.

Proof of Theorem 3.4. Given a fixed positive integer k, let us pick any integer j between 1 and d. We start by showing the following inequality

$$\left|x_j^{(k)} - x_j^{(k-1)}\right| \leq \frac{\xi}{\sqrt{d}} \left\|\boldsymbol{x}^{(k-1)} - \boldsymbol{x}^{(k-2)}\right\|. \tag{3.24}$$

To see this, we may distinguish two cases.

Case I: $x_j^{(k-1)} \neq x_j^{(k)}$. Let us set

$$\beta_j^{(k-1)} = -\frac{1}{2} S_{jj}^{(k-1)} \left(x_j^{(k-1)} - A_j^{(k-1)}\right) - f_{,j}\left(\boldsymbol{x}^{(k-1)}\right), \tag{3.25}$$

and let us introduce the auxiliary function $\varphi : B_r \to \mathbb{R}$ as

$$\varphi(\boldsymbol{x}) = f_{,j}\left(\boldsymbol{x}\right) - \frac{f_{,j}(\boldsymbol{x}^{(k-1)})}{\frac{1}{2} S_{jj}^{(k-1)} (x_j^{(k)} - x_j^{(k-1)})} h(x_j),$$

where

$$h(x_j) := -\frac{1}{2} S_{jj}^{(k-1)} \left(x_j - x_j^{(k)} + \left(x_j^{(k-1)} - A_j^{(k-1)}\right)\right) - f_{,j}\left(x^{(k-1)}\right) - \beta_j^{(k-1)}.$$

Using equation (3.25), it is easy to verify that

$$\begin{aligned} h(x_j^{(k-1)}) &= \frac{1}{2} S_{jj}^{(k-1)} (x_j^{(k)} - x_j^{(k-1)}), \\ h(x_j^{(k)}) &= 0. \end{aligned}$$

Consequently φ satisfies

$$\varphi(\boldsymbol{x}^{(k-1)}) = 0, \qquad \varphi(\boldsymbol{x}^{(k)}) = f_{,j}(\boldsymbol{x}^{(k)}).$$

Also, it is easy to see that

$$\nabla\varphi(\boldsymbol{x}) = \nabla f_{,j}\left(\boldsymbol{x}\right) - \frac{f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)}{x_j^{(k-1)} - x_j^{(k)}} \boldsymbol{e}^{(j)}.$$

Hence, taking into account Assumption M3 and the mean-value theorem applied to φ, we get

$$\begin{aligned} \left| f_{,j}\left(\boldsymbol{x}^{(k)}\right) \right| &= \left| \varphi(\boldsymbol{x}^{(k)}) - \varphi(\boldsymbol{x}^{(k-1)}) \right| \\ &\le \sup_{x \in B} \|\nabla\varphi(\boldsymbol{x})\| \left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \right\| \\ &= \sup_{k\ge 1} \sup_{x\in B} \left\| \nabla f_{,j}\left(\boldsymbol{x}\right) - \frac{f_{,j}\left(\boldsymbol{x}^{(k-1)}\right)}{x_j^{(k-1)} - x_j^{(k)}} \boldsymbol{e}^{(j)} \right\| \left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \right\| \\ &\le \frac{\xi}{M} \left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \right\|. \end{aligned} \tag{3.26}$$

Finally, the above inequality (3.26) together with Lemma 3.7 imply that (3.24) holds true for the case $x_j^{(k-1)} \neq x_j^{(k)}$.

Case II: $x_j^{(k-1)} = x_j^{(k)}$. Then inequality (3.24) obviously holds true in this case as well.

Now, combining inequality (3.24) and employing Lemma 3.7 again we immediately deduce that

$$\left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \right\| \le \xi \left\| \boldsymbol{x}^{(k-1)} - \boldsymbol{x}^{(k-2)} \right\|.$$

Consequently, we have

$$\begin{aligned} \left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(0)} \right\| &= \left\| \sum_{l=1}^{k} \left(\boldsymbol{x}^{(l)} - \boldsymbol{x}^{(l-1)} \right) \right\| \le \sum_{l=1}^{k} \left\| \boldsymbol{x}^{(l)} - \boldsymbol{x}^{(l-1)} \right\| \\ &\le \left(\sum_{l=1}^{k} \xi^{l-1} \right) \left\| \boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)} \right\| \le \frac{1}{1-\xi} \left\| \boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)} \right\|. \end{aligned} \tag{3.27}$$

Applying Lemma 3.7 with $k = 1$ and using Assumption M4, we conclude that

$$\left\| \boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)} \right\| \le r(1-\xi).$$

Combining this with the previous inequality leads to:

$$\left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(0)} \right\| \le r, \tag{3.28}$$

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which shows that each iterate $\boldsymbol{x}^{(k)}$ belongs to the ball B_r. Next, we prove that $\left\{x^{(k)}\right\}$ is a Cauchy sequence, and since $\mathbb{R}^d$ is complete, it has a limit, say $\boldsymbol{x}_*$, in B_r. Indeed, for any integer $k \geq 0$ and $l > 0$, we have

$$\begin{aligned} \left\|\boldsymbol{x}^{(k+l)} - \boldsymbol{x}^{(k)}\right\| &= \left\|\sum_{i=0}^{l-1}\left(\boldsymbol{x}^{(k+i+1)} - \boldsymbol{x}^{(k+i)}\right)\right\| \leq \sum_{i=0}^{l-1}\left\|\boldsymbol{x}^{(k+i+1)} - \boldsymbol{x}^{(k+i)}\right\| \\ &\leq \xi^k \left\|\boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)}\right\| \sum_{i=0}^{l-1}\xi^i \leq \frac{\xi^k}{1-\xi}\left\|\boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)}\right\|. \end{aligned} \tag{3.29}$$

As l goes to infinity in (3.29), we can get more precise estimates than those obtained in (3.27),

$$\left\|\boldsymbol{x}^{(k)} - \boldsymbol{x}_*\right\| \leq \frac{\xi^k}{1-\xi}\left\|\boldsymbol{x}^{(1)} - \boldsymbol{x}^{(0)}\right\|,$$

thus proving that $\{\boldsymbol{x}^{(k)}\}$ converges geometrically to a limit $\boldsymbol{x}_*$. Recalling equation (3.28), we obviously have $\boldsymbol{x}_* \in B_r$. Now, if the sequence $\{\boldsymbol{x}^{(k)}\}$ is convergent to a limit $\boldsymbol{x}_*$ and passing to the limit in equation (3.26), we immediately deduce from the continuity of ∇f that $\nabla f(\boldsymbol{x}_*) = 0$. To complete the proof we show that, under Assumption M3, $\boldsymbol{x}_*$ is the unique stationary point of f in B_r. To this end, assume that there is another point $\tilde{\boldsymbol{x}} \in B_r$ with $\tilde{\boldsymbol{x}} \neq \boldsymbol{x}_*$ and which solves $\nabla f(\boldsymbol{x}) = 0$. We will show that this leads to a contradiction. Since by Assumption M4 we have $f_{,j}(\boldsymbol{x}_0) \neq 0$, Lemma 3.5 with $k = 1$ ensures that $x_j^{(0)} \neq x_j^{(1)}$, for all $j = 1, \ldots, d$. Hence, we may define for each $j = 1, \ldots, d$, the auxiliary function

$$\lambda_j(\boldsymbol{x}) = \frac{x_j^{(1)} - x_j^{(0)}}{f_{,j}(\boldsymbol{x}^{(0)})}\left(f_{,j}(\boldsymbol{x}) - \frac{f_{,j}(\boldsymbol{x}_0)}{x_j^{(0)} - x_j^{(1)}}(x_j - x_{*j})\right).$$

Obviously λ_j simultaneously satisfies $\lambda_j(\boldsymbol{x}_*) = 0$ and $\lambda_j(\tilde{\boldsymbol{x}}) = x_{*j} - \tilde{x}_j$. Therefore, applying again Lemma 3.7 for $k = 1$, we get from the mean value theorem and (3.20),

$$\begin{aligned} |x_{*j} - \tilde{x}_j| = |\lambda_j(\boldsymbol{x}_*) - \lambda_j(\tilde{\boldsymbol{x}})| &\leq \sup_{x \in B}\|\nabla\lambda_j(\boldsymbol{x})\|\,\|\tilde{\boldsymbol{x}} - \boldsymbol{x}_*\| \\ &= \left|\frac{x_j^{(1)} - x_j^{(0)}}{f_{,j}(\boldsymbol{x}^{(0)})}\right| \sup_{x \in B}\left\|\nabla f_{,j}(\boldsymbol{x}) - \frac{f_{,j}\left(\boldsymbol{x}^{(0)}\right)}{x_j^{(0)} - x_j^{(1)}}\boldsymbol{e}^{(j)}\right\|\,\|\tilde{\boldsymbol{x}} - \boldsymbol{x}_*\| \\ &\leq \frac{\xi}{\sqrt{d}}\|\tilde{\boldsymbol{x}} - \boldsymbol{x}_*\|. \end{aligned}$$

Then, we immediately obtain that

$$0 < \|\tilde{\boldsymbol{x}} - \boldsymbol{x}_*\| \leq \xi\,\|\tilde{\boldsymbol{x}} - \boldsymbol{x}_*\|$$

with $\xi \in (0, 1)$, and therefore the last inequality holds only if $\tilde{\boldsymbol{x}} = \boldsymbol{x}_*$, which is clearly a contradiction. Hence, we can conclude that f has a unique stationary point. Thus, the theorem is proved. $\square$

We conclude this section by giving a simple one-dimensional example, which illustrates the performance of our method by showing that it has a wider convergence domain than the classical Newton's method.

EXAMPLE 3.8. Consider the function $f : \mathbb{R} \to \mathbb{R}$ defined by

$$f(x) = -e^{-x^2}.$$

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TABLE 3.1
The MMA convergence: $f(x) = -e^{-x^2}$.

Iteration	x	$f'(x)$
0	7.071^{-1}	8.578^{-1}
1	9.250^{-5}	1.850^{-4}
2	5.341^{-5}	1.068^{-4}
3	3.083^{-5}	6.167^{-5}
4	1.780^{-5}	3.561^{-5}
5	1.028^{-5}	2.056^{-5}
6	5.934^{-6}	1.187^{-5}
7	3.426^{-6}	6.852^{-6}
8	1.978^{-6}	3.956^{-6}
9	1.142^{-6}	2.284^{-6}
10	6.594^{-7}	1.319^{-6}

Its first and second derivatives are given, respectively, by

$$f'(x) = 2xe^{-x^2}, \qquad f''(x) = 2\left(1-2x^2\right)e^{-x^2}.$$

Since the second derivative of f is positive in the interval $\left]-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right[$, Newton's method shall converge to the minimum of f.

Let us recall that the famous Newton's method for finding x_* uses the iterative scheme $\left\{x^{(k)}\right\}$ defined by

$$x^{(k+1)} = x^{(k)} - \frac{f'\left(x^{(k)}\right)}{f''\left(x^{(k)}\right)}, \qquad \forall k \geq 0,$$

starting from some initial value $x^{(0)}$. It converges quadratically in some neighborhood of x_* for a simple root x_*. In our example, the Newton iteration becomes

$$x^{(k+1)} = x^{(k)}\left(1 - \frac{1}{1-2(x^{(k)})^2}\right), \qquad k \geq 0.$$

Starting from the initial approximation $x^{(0)} = \frac{1}{2}$ (respectively $x^{(0)} = -\frac{1}{2}$), the Newton iterates are given by $x^{(k)} = \frac{1}{2}(-1)^k$ (respectively $x^{(k)} = \frac{1}{2}(-1)^{k+1}$), and hence the sequence $\{x^{(k)}\}$ does not converge. Also for initial values belonging to the interval $]-\frac{1}{\sqrt{2}}, -\frac{1}{2}[\cup]\frac{1}{2}, \frac{1}{\sqrt{2}}[$, after some iteration, the sequence lies outside the interval $]-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}[$ and diverges. The domain of convergence of Newton's method is only the interval $]-\frac{1}{2}, \frac{1}{2}[$.

Differently from the Newton's method, it is observed that our MMA method converges for any initial value taken in the larger interval $]-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}[$. Convergence results are reported in Table 3.1.

4. A multistage turbine using a through-flow code. The investigation of through-flow have been used for many years in the analysis and the design of turbomachineries by many authors, especially in the seventies; see for example [8, 19, 31]. The main ideas in these investigations are based on the numerical analysis of the stream line curvatures and the matrix

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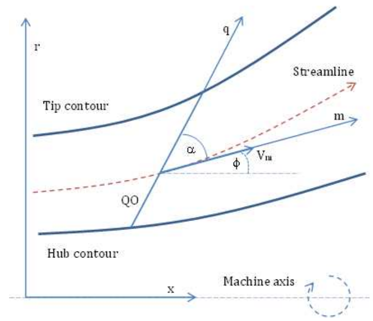

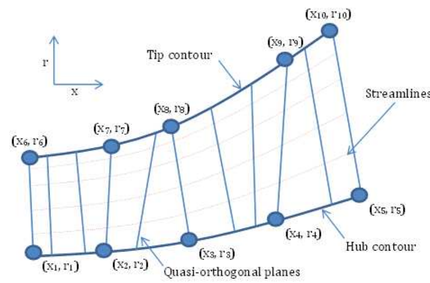

FIG. 4.1. *Meridional view of the flow path (left panel), and Steam path design geometry (right panel).*

through-flow. More details can be found in [6, 7, 9, 17, 20, 21]. The stream line curvature method offers a flexible way of determining an Euler solution of an axisymmetric flow through a turbomachine. The theory of stream line curvature through-flow calculations has been described by many authors, particularly by John Denton [7]. From the assumption of axial symmetry, it is possible to define a series of meridional stream surfaces, a surface of revolution along which particles are assumed to move through the machine. The principle of stream line curvature is to express the equation of motion along lines roughly perpendicular to these stream surfaces (quasi-orthogonal lines) in terms of the curvature of the surfaces in the meridional plane, as shown in the left panel of Figure 4.1. The two unknowns indicate that we are interested in the meridional fluid component of the velocity V_m ($^{\mathrm{m}}/_{\mathrm{s}}$) in the direction of the stream lines and the mass flow rate $\dot{m}$ ($^{\mathrm{kg}}/_{\mathrm{s}}$).

The mass flow rate is evaluated at each location point at the intersections of the stream lines and the quasi-orthogonal lines, and it also depends on the variation of the meridional fluid velocity V_m. The continuity equation takes the form

$$\dot{m} = 2\pi \int_{r_{hub}}^{r_{tip}} r\rho V_m\,(q,m)\sin\alpha\,(1-b)\,dq, \tag{4.1}$$

where $0 \le b < 1$ is the blade blockage factor, r the radius of the rotating machine axis (m), and ρ the fluid density ($^{\mathrm{kg}}/_{\mathrm{m}^3}$). The inlet mass flow rate is the mass flow rate calculated along the first quasi-orthogonal line.

Knowing the geometrical lean angle of the blades, i.e., the inclination of the blades in the tangential direction ε (rad), the total enthalpy H $(\mathrm{N.m})$, the static temperature T (K), and the entropy S ($^{\mathrm{J}}/_{\mathrm{K}}$) as input data functions evaluated by empirical rules, we can find the variation of the meridional fluid velocity V_m as a function of the distance q (m) along the quasi-orthogonal lines and the meridional direction by solving the equilibrium equation

$$\begin{aligned}\frac{1}{2}\frac{dV_m^2\,(q,m)}{dq} &= \frac{V_m^2\,(q,m)}{r_c}\sin\alpha + V_m\frac{\partial V_m\,(q,m)}{\partial m}\cos\alpha - \frac{1}{2r_c}\frac{d\left(r^2V_\theta^2\,(q,m)\right)}{dq}\\ &\quad + \frac{dH\,(q,m)}{dq} - T\frac{dS\,(q,m)}{dq}\\ &\quad - \tan\varepsilon\frac{V_m}{r}\frac{\partial\,(rV_\theta)}{\partial m},\end{aligned}$$

where θ represents the direction of rotation, and the values of rV_θ are specified while operating the design mode. The angle α (rad) between the quasi-orthogonal lines and the stream surface, and the radius of curvature r_c (m) are updated with respect to the mass flow rate

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distribution $\dot{m}$ ($^{\mathrm{kg}}/_{\mathrm{s}}$) . The enthalpy is updated according to the IAPWS-IF97 steam function as described in [29]. The entropy is calculated by fundamental thermodynamic relations between the internal energy of the system and external parameters (e.g., friction losses).

The computational parameters of the stream lines are drawn in a meridional view of the flow path in the left panel of Figure 4.1 with one of the quasi-normal stations that are strategically located in the flow between the tip and hub contours. Several stations are generally placed in the inlet duct upstream of the turbomachine, the minimum number of quasi-orthogonal stations between the adjacent pair of blade rows is simply one, which characterizes both outlet conditions from the previous row and inlet conditions to the next. In our stream line curvature calculation tool, there is one quasi-orthogonal station at each edge of each blade row. Given these equations and a step-by-step procedure, we obtain a solution as described in [22].

In the left panel of Figure 4.2, the contour of the turbomachine is limited on the top by the line that follows the tip contour at the casing and on the bottom by a line that follows the geometry of the hub contour at the rotor. Intermediate lines are additional stream lines, distributed according to the mass flow rate that goes through the stream tubes. Vertical inclined lines are the quasi-orthogonal stations mainly located at the inlet and outlet of moving and fixed blade rows.

The possibility to impose a target mass flow rate at the inlet of the turbomachine is very important for its final design as it is driven by downstream conditions. Equation (4.1) shows that the mass flow rate depends explicitly on the shape of the turbomachine through the position of the extreme points r_{hub} and r_{tip} of the quasi-orthogonal lines. The purpose of our inverse problem is to identify both hub and tip contours of the turbomachine to achieve an expected mass flow rate at the inlet of the turbomachine.

The geometry of the contours of the turbomachine is defined by a univariate interpolation of n points along the r-axis. The interpolation is based on the improved method developed by Hiroshi Akima [1]. In this method, the interpolating function is a piecewise polynomial function composed of a set of polynomials defined at successive intervals of the given data points. We use the third-degree polynomial default option as it is not required to reduce any undulations in the resulting curves.

In this realistic example, we use five points on each curve describing, respectively, the hub and the tip contours; see the right panel of Figure 4.2. The initial ten data points are extracted from an existing geometry and are chosen arbitrary equidistant along the axial direction. Their radial position is linearly interpolated using the two closest points. The unconstrained optimization will be to find $\boldsymbol{r}_* = (r_{*,1}, r_{*,2}, \ldots, r_{*,10})^\top \in \mathbb{R}^{10}$ such that

$$f(\boldsymbol{r}_*) = \min_{\boldsymbol{r}\in\mathbb{R}^{10}} f(\boldsymbol{r}), \tag{4.2}$$

where $f(\boldsymbol{r}) := \left(\frac{\underline{\dot{m}} - \dot{m}(\boldsymbol{r})}{\underline{\dot{m}}}\right)^2$, $\dot{m}(\boldsymbol{r})$ is the mass flow rate that depends on the design parameters and $\underline{\dot{m}}$ is the imposed inlet mass flow rate.

In our example, the target inlet mass flow rate is $\underline{\dot{m}} = 200\ ^{\mathrm{kg}}/_{\mathrm{s}}$, and the initial realistic practical geometry gives an initial mass flow rate of $\dot{m}_0 = 161.20\ ^{\mathrm{kg}}/_{\mathrm{s}}$ with

$$r_0 = (0.828, 0.836, 0.853, 0.853, 0.853, 0.962, 1.05, 1.337, 1.701, 2.124)^T.$$

The difference between the target and the initial inlet mass flow value is about 20% which is considered to be very significant in practice. The initial shape is shown in the left panel of Figure 4.2.

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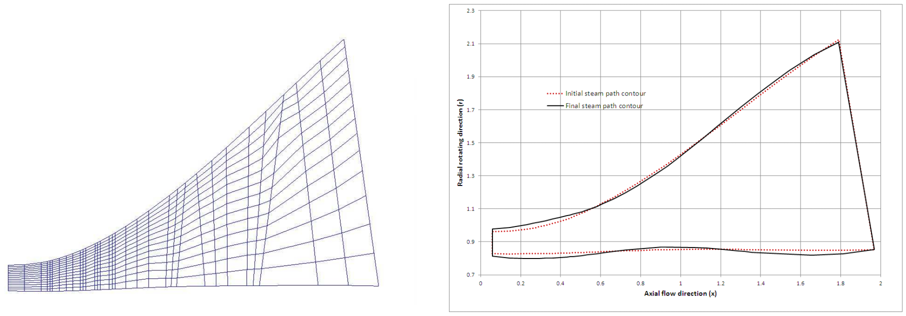

FIG. 4.2. *Initial steam path contour (left panel), and Initial and optimized steam path contours (right panel).*

The moving asymptotes are chosen such that the condition (3.15) is automatically satisfied, and their numerical implementation is defined by

$$A_j^{(k)} = \begin{cases} L_j^{(k)} = r_j^{(k)} + 4\dfrac{f_{,j}\left(\boldsymbol{r}^{(k)}\right)}{S_{jj}^{(k)}} & \text{if } f_{,j}\left(\boldsymbol{r}^{(k)}\right) < 0, \\ U_j^{(k)} = r_j^{(k)} + 4\dfrac{f_{,j}\left(\boldsymbol{r}^{(k)}\right)}{S_{jj}^{(k)}} & \text{if } f_{,j}\left(\boldsymbol{r}^{(k)}\right) > 0. \end{cases}$$

It is important to note the simple form which is used here for the selection of the moving asymptotes. The first-order partial derivatives are numerically calculated using a two-point formula that computes the slope

$$\frac{f\left(r_1, \dots, r_j + h, \dots, r_{10}\right) - f\left(r_1, \dots, r_j - h, \dots, r_{10}\right)}{2h}, \quad j = 1, \dots, 10,$$

with an error of order h^2. For our numerical study, h has been chosen equal to $5 \cdot 10^{-4}$ that corresponds to about $5 \cdot 10^{-2}$ % of the size of the design parameters, which gives an approximation accurate enough. To avoid computing second-order derivatives of the objective function f, we use the spectral parameter as defined in (3.9). We observe a good convergence to the target inlet mass flow rate displayed in Table 4.1. The final stream path geometry is compared with the initial geometry in the right panel of Figure 4.2, where the optimized hub and tip contour values are

$$r_* = (0.824, 0.821, 0.857, 0.851, 0.853, 0.966, 1.074, 1.331, 1.703, 2.124)^T.$$

It appears that the hub contour of the optimized shape is more deformed than the tip contour, and the shape is more sensitive to the design parameters of the hub than the tip contours.

5. Concluding remarks. In this paper we develop and analyze new local convex approximation methods with explicit solutions of non-linear problems for unconstrained optimization for large-scale systems and in the framework of the structural mechanical optimization of multi-scale models based on the moving asymptotes algorithm (MMA).We show that the problem leads us to use second derivative information in order to solve more efficiently structural optimization problems without constraints. The basic idea of our MMA methods can be interpreted as a technique that approximates a priori the curvature of the object function. In order to avoid second derivative evaluations in our algorithm, a sequence of diagonal Hessian estimates, where only the first- and zeroth-order information is accumulated during the previous iterations, is used. As a consequence, at each step of the iterative process, a strictly convex approximation subproblem is generated and solved. A convergence

TABLE 4.1
The convergence of inlet mass flow rate: $\dot{m}$ ($^{\mathrm{kg}}/_{\mathrm{s}}$) in the optimization problem (4.2) to the target inlet mass flow $\underline{\dot{m}} = 200\ ^{\mathrm{kg}}/_{\mathrm{s}}$.

Iteration	Inlet mass flow rate: $\dot{m}$ (kg/s)	Objective function: $f(\boldsymbol{r})$
0	162.10	0.359010^{-1}
1	170.42	0.218812^{-1}
2	178.54	0.115096^{-1}
3	186.51	0.455025^{-2}
4	194.32	0.806159^{-3}
5	201.74	0.752755^{-4}
6	199.50	0.636189^{-5}
7	200.26	0.167331^{-5}
8	199.97	0.170603^{-7}
9	200.10	0.232201^{-6}
10	199.99	0.366962^{-8}

result under fairly mild assumptions, which takes into account the second-order derivatives information for our optimization algorithm, is presented in detail.

It is shown that the approximation scheme meets all well-known properties of the MMA such as convexity and separability. In particular, we have the following major advantages:

- All subproblems have *explicit* solutions. This considerably reduces the computational cost of the proposed method.
- The method generates an iteration sequence, that, under mild technical assumptions, is bounded and converges geometrically to a stationary point of the objective function with one or several variables from any ”good” staring point.

The numerical results and the theoretical analysis of the convergence are very promising and indicate that the MMA method may be further developed for solving general large-scale optimization problems. The methods proposed here also can be extended to more realistic problems with constraints. We are now working to extend our approach to constrained optimization problems and investigate the stability of the algorithm for some reference cases described in [32].

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REFERENCES

[1] H. AKIMA, *A new method of interpolation and smooth curve fitting based on local procedures*, J. ACM, 17 (1970), pp. 589–602.
[2] K.-U. BLETZINGER, *Extended method of moving asymptotes based on second-order information*, Struct. Optim., 5 (1993), pp. 175–183.
[3] S. BOYD AND L. VANDENBERGHE, *Convex Optimization*, Cambridge University Press, Cambridge, 2004.
[4] M. BRUYNEEL, P. DUYSINX, AND C. FLEURY, *A family of MMA approximations for structural optimization*, Struct. Multidiscip. Optim., 24 (2002), pp. 263–276.

[1]ALSTOM Ltd., Brown Boveri Strasse 10, CH-5401 Baden, Switzerland (roland.simmen@power.alstom.com)

[5] H. CHICKERMANE AND H. C. GEA, *Structural optimization using a new local approximation method*, Internat. J. Numer. Methods Engrg., 39 (1996), pp. 829–846.
[6] C. CRAVERO AND W. N DAWES, *Throughflow design using an automatic optimisation strategy*, in ASME Turbo Expo, Orlando 1997, paper 97-GT-294, ASME Technical Publishing Department, NY, 1997.
[7] J. D. DENTON, *Throughflow calculations for transonic axial flow turbines*, J. Eng. Gas Turbines Power, 100 (1978), pp. 212–218.
[8] ———, *Turbomachinery Aerodynamics, Introduction to Numerical Methods for Predicting Turbomachinery Flows*, University of Cambridge Program for Industry, 21st June, 1994.
[9] J. D. DENTON AND CH. HIRSCH, *Throughflow calculations in axial turbomachines*, AGARD Advisory report No. 175, AGARD, Neuilly-sur-Seine, France, 1981.
[10] R. FLETCHER, *Practical Methods of Optimization*, 2nd. ed., Wiley, New York, 2002.
[11] C. FLEURY, *Structural optimization methods for large scale problems: computational time issues*, in Proceedings WCSMO-8 (Eighth World Congress on Structural and Multidisciplinary Optimization), Lisboa/Portugal, 2009.
[12] ———, *Efficient approximation concepts using second order information*, Internat. J. Numer. Methods Engrg., 28 (1989), pp. 2041–2058.
[13] ———, *First and second order convex approximation strategies in structural optimization*, Struct. Optim., 1 (1989), pp. 3–11.
[14] C. FLEURY AND V. BRAIBANT, *Structural optimization: A new dual method using mixed variables*, Internat. J. Numer. Methods Engrg., 23 (1986), pp. 409–428.
[15] M. A GOMES-RUGGIERO, M. SACHINE, AND S. A. SANTOS, *Solving the dual subproblem of the methods of moving asymptotes using a trust-region scheme*, Comput. Appl. Math., 30 (2011), pp. 151–170.
[16] ———, *A spectral updating for the method of moving asymptotes*, Optim. Methods Softw., 25 (2010), pp. 883–893.
[17] H. MARSH, *A digital computer program for the through-flow fluid mechanics in an arbitrary turbomachine using a matrix method*, tech. report, aeronautical research council reports and memoranda, No. 3509, 1968.
[18] Q. NI, *A globally convergent method of moving asymptotes with trust region technique*, Optim. Methods Softw., 18 (2003), pp. 283–297.
[19] R. A. NOVAK, *Streamline curvature computing procedures for fluid-flow problems*, J. Eng. Gas Turbines Power, 89 (1967), pp. 478–490.
[20] P. PEDERSEN, *The integrated approach of fem-slp for solving problems of optimal design*, in Optimization of Distributed Parameter Structures vol. 1., E. J. Haug and J. Gea, eds., Sijthoff and Noordhoff, Alphen a. d. Rijn, 1981, pp. 757–780.
[21] M. V. PETROVIC, G. S. DULIKRAVICH, AND T. J. MARTIN, *Optimization of multistage turbines using a through-flow code*, Proc. Inst. Mech. Engrs. Part A, 215 (2001), pp. 559–569.
[22] M. T. SCHOBEIRI, *Turbomachinery Flow Physics and Dynamic Performance*, Springer, New York, 2012.
[23] H. SMAOUI, C. FLEURY, AND L. A. SCHMIT, *Advances in dual algorithms and convex approximation methods*, in Procceedings of AIAA/ASME/ASCE 29th Structures, Structural Dynamics, and Materials Conference, Williamsburg, AIAA, Reston, VA, 1988, pp. 1339–1347.
[24] K. SVANBERG, *MMA and GCMMA, version September 2007*, technical note, KTH, Stockholm, Sweden, 2007. http://www.math.kth.se/ krille/gcmma07.pdf.
[25] ———, *A class of globally convergent optimization methods based on conservative convex separable approximations*, SIAM J. Optim., 12 (2002), pp. 555–573.
[26] ———, *The method of moving asymptotes, modelling aspects and solution schemes*, Lecture notes for the DCAMM course Advanced Topics in Structural Optimization, Lyngby, June 25 - July 3, Springer, 1998.
[27] ———, *A globally convergent version of mma without linesearch*, in Proceedings of the First World Congress of Structural and Multidisciplinary Optimization, N. Olhoff and G. I. N. Rozvany, eds., Pergamon, Oxford, 1995, pp. 9–16.
[28] ———, *The method of moving asymptotes—a new method for structural optimization*, Internat. J. Numer. Methods Engrg., 24 (1987), pp. 359–373.
[29] W. WAGNER AND A. KRUSE, *Properties of Water and Steam*, Springer, Berlin, 1998.
[30] H. WANG AND Q. NI, *A new method of moving asymptotes for large-scale unconstrained optimization*, Appl. Math. Comput., 203 (2008), pp. 62–71.
[31] D. H. WILKINSON, *Stability, convergence, and accuracy of 2d streamline curvature methods*, Proc. Inst. Mech. Engrs., 184 (1970), pp. 108–119.
[32] D. YANG AND P. YANG, *Numerical instabilities and convergence control for convex approximation methods*, Nonlinear Dynam., 61 (2010), pp. 605–622.
[33] W. H. ZHANG AND C. FLEURY, *A modification of convex approximation methods for structural optimization*, Comput. & Structures, 64 (1997), pp. 89–95.
[34] C. ZILLOBER, *Global convergence of a nonlinear programming method using convex approximations*, Numer. Algorithms, 27 (2001), pp. 265–289.