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MULTIVARIATE PADÉ APPROXIMATION AND ITS APPLICATION IN SOLVING SYSTEMS OF NONLINEAR EQUATIONS*1)

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Abstract

For a certain kind of multivariate Padé approximation problems, we establish in this paper some results about the solvability and uniqueness of its solution. We give also the necessary and sufficient conditions for the continuity of Padé approximation operator. The application of such approximants in finding solutions of systems of nonlinear equations is considered, and some numerical examples are given, in which it is shown that the Padé methods are more effective than the Newton methods in some cases.

§1. Introduction

It is well known that univariate Padé approximation(UPA) is a useful tool as rational approximants to a specified power series and has numerous applications in the fields of numerical analysis, theoretical physics and many other subjects(see [1],[2]). The extensions of UPA to the bivariate and multivariate cases were first considered by Chisholm [3] and then followed by Hughes [6],[7], Lutterodt [9],[10], Karlsson and Wallin [8], Cuyt [5] and others. There are numerous possibilities for the extension and generalization by requiring the rational approximants to have certain special properties. Several different definitions for multivariate Padé approximants(MPA) were introduced and much research work was done in the past decade. For a general review on this subject we refer to references [2],[4],[5].

To start with, we introduce some notations. Given a positive integer n, we write $\mathbf{Z}_+^n = \{\alpha : \alpha = [\alpha_1, \cdots, \alpha_n]^T, \alpha_i \in \mathbf{Z}_+, i = 1, \cdots, n\}$, where $\mathbf{Z}_+$ denote the set of all nonnegative integers. The set $\mathbf{Z}_+^n$ is often referred to as the set of multi-indices. Given two vectors $\mathbf{a}$ and $\mathbf{b}$ in $\mathbf{R}$, we shall use the standard notations $\mathbf{a} \le \mathbf{b}$ if and only if $a_i \le b_i, i = 1, \cdots, n$, $\mathbf{a} + \mathbf{b} = [a_1 + b_1, \cdots, a_n + b_n]^T$. If $\alpha \in \mathbf{Z}_+^n, \mathbf{x} \in \mathbf{R}^n$, we write $|\alpha| = \sum_{i=1}^n \alpha_i$, $\|\mathbf{x}\| = \sqrt{\sum_{i=1}^n x_i^2}$ and $\mathbf{x}^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. We also use the notations $0 = [0, \cdots, 0]^T$, $1 = [1, \cdots, 1]^T$ and $\mathbf{e}_i$ = unit vector in the i-th direction $= [0, \cdots, 1, \cdots, 0]^T$.

The general framework of the definition for MPA to a given function $f(\mathbf{x}) = \sum_{\alpha \in \mathbf{Z}_+^n} c_\alpha \mathbf{x}^\alpha$ consists of choosing three multi-index sets N, D and E in $\mathbf{Z}_+^n$ and finding two polynomials $p(\mathbf{x}) = \sum_{\alpha \in N} a_\alpha \mathbf{x}^\alpha$, $q(\mathbf{x}) = \sum_{\alpha \in D} b_\alpha \mathbf{x}^\alpha$, such that $p(\mathbf{x}) - f(\mathbf{x}) q(\mathbf{x}) = \sum_{\alpha \in \mathbf{Z}_+^n \setminus E} e_\alpha \mathbf{x}^\alpha$, $q(0) = 1$.

In the case of UPA, the problem of $(m/l)_f$ Padé approximants is to take $N = \{0, 1, \cdots, m\}$, $D = \{0, 1, \cdots, l\}$ and $E = \{0, 1, \cdots, m + l\}$. However, in the multivariate case, N, D and E can be taken in various manners. Therefore, there may be many different definitions

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for MPA (see [3]–[10]). For the general framework (1.1) of MPA, it is difficult to give simple and easily used conditions under which the existence and uniqueness of MPA are guaranteed. In this paper, we choose N, D and E as follows

$$N = \{\alpha : \alpha \in \mathbf{Z}_+^n,\ |\alpha| \le 1\}, \tag{1.2}$$

$$D = \{\alpha : \alpha \in \mathbf{Z}_+^n,\ |\alpha| \le k,\ \alpha \ne k\mathbf{e}_i,\ i = 1, \cdots, n\}, \tag{1.3}$$

$$E = \{\alpha : \alpha \in \mathbf{Z}_+^n,\ |\alpha| \le k\}, \tag{1.4}$$

where $k \ge 2$. For such N, D and E we study the existence of MPA in §2. The problem of uniqueness is considered in §3. In §4, we investigate the problem of the continuity of Padé approximation operators. In the last section, we consider the problem of application of MPA in solving systems of nonlinear equations.

§2. Existence

For N, D and E defined as in (1.2)–(1.4), let $p(\mathbf{x}) = a_0 + \sum_{|\alpha|=1} a_\alpha \mathbf{x}^\alpha$, $q(\mathbf{x}) = 1 + \sum_{\alpha \in D\setminus\{0\}} b_\alpha \mathbf{x}^\alpha$, Then equation (1.1) is equivalent to the following

$$a_0 = c_0, \quad a_\alpha = c_\alpha + b_\alpha c_0, \quad \alpha \in N \setminus \{0\}, \tag{2.1}$$

$$\sum_{\substack{\alpha+\beta=\gamma \\ \beta \in D\setminus\{0\}}} c_\alpha b_\beta + c_\gamma = 0, \quad \gamma \in E \setminus N. \tag{2.2}$$

Equations (2.1)–(2.2) are linear systems with $|E|$ ($|E|$ stands for the cardinality of E) unknowns and $|E|$ equations. Therefore it is expected to have the unique solution.

Take $\alpha = \mathbf{e}_i$ in (2.1), $\gamma = j\mathbf{e}_i$, $j = 2, \cdots, k$, in (2.2); equations (2.1)–(2.2) have the following equations as their sub–equations

$$a_0 = c_0, \quad a_1^{(i)} = c_1^{(i)} + b_1^{(i)} c_0, \tag{2.3}$$

$$\sum_{s+t=j} c_s^{(i)} b_t^{(i)} + c_j^{(i)} = 0, \quad j = 2, \cdots, k,$$

where $a_1^{(i)} = a_{\mathbf{e}_i}$, $b_t^{(i)} = b_{t\mathbf{e}_i}$, $c_s^{(i)} = c_{s\mathbf{e}_i}$, and $i = 1, \cdots, n$. It is not hard to see that equations (2.3) are the Padé equations for UPA $(1/k-1)_{g_i}$ with $g_i = f(x\mathbf{e}_i)$. Hence problem (1.1) is connected closely with UPA $(1/k-1)_{g_i}$, $i = 1, \cdots, n$. Suppose equations (2.1)–(2.2) are solvable; then (2.3) are solvable also for $i = 1, \cdots, n$. From the theory of the UPA [14], it follows that

$$\text{rank } H_i(1, k-2, k-2) = \text{ rank } H_i(2, k-1, k-2), \quad i = 1, \cdots, n, \tag{2.4}$$

where

$$H_i(m, j, k) = \begin{bmatrix} c_m^{(i)} & c_{m-1}^{(i)} & \cdots & c_{m-j}^{(i)} \\ c_{m+1}^{(i)} & c_m^{(i)} & \cdots & c_{m-j+1}^{(i)} \\ \cdots & \cdots & \cdots & \cdots \\ c_{m+k}^{(i)} & c_{m+k-1}^{(i)} & \cdots & c_{m+k-j}^{(i)} \end{bmatrix}, \quad i = 1, \cdots, n.$$

Hence relations (2.4) are necessary conditions for the solvability of (2.1)–(2.2). Now we shall show that if $c_0 \ne 0$, these conditions are also sufficient. In fact, from (2.2) we have

$$b_\gamma = -c_0^{-1} \sum_{\substack{\alpha+\beta=\gamma \\ \alpha\ne 0, \beta \in D}} c_\alpha b_\beta, \quad \gamma \in D \setminus \{0\}. \tag{2.5}$$

Therefore, if $b_t^{(i)} (t = 1, \cdots, k-1,\ i = 1, \cdots, n)$ satisfy equations (2.3), then b_γ can be determined recursively by (2.5) from $b_t^{(i)}$. Hence (2.1)–(2.2) are solvable. Thus we have established the main part of the following theorem.

Theorem 2.1. *Padé approximation problem* (1.1) *is solvable if and only if one of the following two conditions is satisfied:* 1) $c_0 = 0$ *and the equation*

$$\sum_{\substack{\alpha+\beta=\gamma \\ \alpha\neq 0 \\ \beta\in D\setminus\{0\}}} c_\alpha b_\beta + c_\gamma = 0, \quad \gamma \in E \setminus N \tag{2.6}$$

is solvable. 2) $c_0 \neq 0$ *and*

$$\text{rank } H_i(1, k-2, k-2) = \text{ rank } H_i(2, k-1, k-2), \quad i = 1, \cdots, n. \tag{2.7}$$

Proof. For $c_0 \neq 0$, the validity of the theorem is proved already. If $c_0 = 0$, equation (2.6) follows from (2.2). So the theorem is true.

Corollary 2.1. Let $k = 2$. Then Padé approximation problem (1.1) is solvable if and only if one of the following two conditions is satisfied: 1) $c_0 = 0$ and

$$\frac{c_2^{(i)}}{c_1^{(i)2}} + \frac{c_2^{(j)}}{c_1^{(j)2}} = \frac{c_2^{(i,j)}}{c_1^{(i)}c_1^{(j)}} \quad \text{for} \quad c_1^{(i)}c_1^{(j)} \neq 0,\ i \neq j, \tag{2.8}$$

$$c_2^{(i,j)} = 0 \quad \text{for} \quad c_1^{(i)} = c_1^{(j)} = 0, \tag{2.9}$$

$$\frac{c_2^{(i,j)}}{c_1^{(j)}} = \text{const.} \quad \text{for any } i \text{ such that } c_1^{(i)} = 0 \quad \text{and fixed } j \text{ with } c_1^{(j)} \neq 0. \tag{2.10}$$

2) $c_0 \neq 0$ and

$$c_2^{(i)} = 0 \quad for \quad c_1^{(i)} = 0, \tag{2.11}$$

where $c_m^{(i_1,\cdots,i_m)} = c_{e_{i_1}+\cdots+e_{i_m}}$.

Proof. 1) Take $\gamma = 2\,\mathbf{e}_i$; then (2.6) implies

$$c_1^{(i)}b_1^{(i)} + c_2^{(i)} = 0, \quad i = 1, \cdots, n. \tag{2.12}$$

Hence $c_2^{(i)} = 0$ for $c_1^{(i)} = 0$. Take $\gamma = \mathbf{e}_i + \mathbf{e}_j$, $i \neq j$; then (2.6) implies

$$c_1^{(i)}b_1^{(j)} + c_1^{(j)}b_1^{(i)} + c_2^{(i,j)} = 0. \tag{2.13}$$

If $c_1^{(i)}c_1^{(j)} \neq 0$, then (2.12) and (2.13) imply (2.8). If $c_1^{(i)} = c_1^{(j)} = 0$, then we have from (2.13) that $c_2^{(i,j)} = 0$. This is (2.9). If $c_1^{(i)} = 0, c_1^{(j)} \neq 0$, then (2.13) implies (2.10).

2) If $c_0 \neq 0$, then relation (2.11) follows from (2.7).

Concerning computation of MPA, we suppose $c_0 \neq 0$; then relation (2.5) can be used to compute b_β for $|\beta| > 1$. If $|\beta| = 1$, b_β can be obtained by solving UPA problem $(1/k-1)_{g_i}$. It is well known that several efficient methods can be used. The most simple and effective method may be Baker algorithm [2].

For the application in §5, we need to compute the numerator $p(\mathbf{x}) = a_0 + \sum_{i=1}^n a^{(i)}x_i$ For $k \leq 4$ the explicit formulas for a_i are given as follows

$$k = 2, \quad a_i = c_1^{(i)} - c_0\frac{c_2^{(i)}}{c_1^{(i)}}, \quad i = 1, \cdots, n.$$

$$k=3,\quad a_i=c_1^{(i)}-c_0\frac{c_3^{(i)}-c_1^{(i)}c_2^{(i)}}{c_0c_2^{(i)}-c_1^{(i)^2}},\quad i=1,\cdots,n.$$

$$k=4,\quad a_i=c_1^{(i)}-c_0\frac{c_0c_1^{(i)}c_3^{(i)}+c_0c_2^{(i)^2}-c_1^{(i)^2}c_2^{(i)}-c_0^2c_4^{(i)}}{2c_0c_1^{(i)}c_2^{(i)}-c_1^{(i)^3}-c_0^2c_3^{(i)}},\quad i=1,\cdots,n.$$

§3. Uniqueness of MPA

For any two solutions $\frac{p(\mathbf{x})}{q(\mathbf{x})}=\sum_{\alpha\in N}a_\alpha\mathbf{x}^\alpha/\sum_{\beta\in D}b_\beta\mathbf{x}^\beta$, and $\frac{p'(\mathbf{x})}{q'(\mathbf{x})}=\sum_{\alpha\in N}a'_\alpha\mathbf{x}^\alpha/\sum_{\beta\in D}b'_\beta\mathbf{x}^\beta$. of problem (1.1), if we always have $p/q=p'/q'$, then we say that the solution of (1.1) is unique. In this section, we shall give the conditions under which the uniqueness is guaranteed.

Since the uniqueness is equivalent to

$$\Big(\sum_{\alpha\in N}a_\alpha\mathbf{x}^\alpha\Big)\Big(\sum_{\beta\in D}b'_\beta\mathbf{x}^\beta\Big)=\Big(\sum_{\alpha\in N}a'_\alpha\mathbf{x}^\alpha\Big)\Big(\sum_{\beta\in D}b_\beta\mathbf{x}^\beta\Big),\quad \mathbf{x}\in\mathbf{R}^n,\tag{3.1}$$

we get

$$(a_0b'_\gamma-a'_0b_\gamma)+\sum_{\substack{\alpha+\beta=\gamma\\ \alpha\in N\setminus\{0\},\beta\in D}}(a_\alpha b'_\beta-a'_\alpha b_\beta)=0,\quad |\gamma|\le k+1.\tag{3.2}$$

By (1.1) we have $p(\mathbf{x})q'(\mathbf{x})-p'(\mathbf{x})q(\mathbf{x})=\sum_{\alpha\notin E}\tilde{e}_\alpha\mathbf{x}^\alpha$. Then (3.2) is always true for $|\gamma|\le k$. From (2.1), relation (3.2) is equivalent to

$$c_0(b'_\gamma-b_\gamma)+\sum_{\substack{\alpha+\beta=\gamma\\ \alpha\in N\setminus\{0\},\beta\in D}}[c_0(b_\alpha b'_\beta-b'_\alpha b_\beta)+c_\alpha(b'_\beta-b_\beta)]=0,\quad |\gamma|\le k+1.\tag{3.3}$$

From (2.2), one has $c_0(b'_\gamma-b_\gamma)+\sum_{\substack{\alpha+\beta=\gamma\\ \alpha\ne0,\beta\in D\setminus\{0\}}}c_\alpha(b'_\beta-b_\beta)=0,\quad \gamma\in E\setminus N$. Substituting it into (3.3), we have

$$\sum_{\substack{\alpha+\beta=\gamma\\ \alpha\in N\setminus\{0\},\beta\in D\setminus\{0\}}}c_0(b_\alpha b'_\beta-b'_\alpha b_\beta)-\sum_{\substack{\alpha+\beta=\gamma\\ |\alpha|>1,\beta\in D\setminus\{0\}}}c_\alpha(b'_\beta-b_\beta)=0,\quad \gamma\in E\setminus N,\tag{3.4}$$

and

$$\Delta\equiv\sum_{\substack{\alpha+\beta=\gamma\\ \alpha\in N\setminus\{0\},\beta\in D\setminus\{0\}}}[c_0(b_\alpha b'_\beta-b'_\alpha b_\beta)+c_\alpha(b'_\beta-b_\beta)]=0,\quad |\gamma|=k+1.\tag{3.5}$$

Therefore the uniqueness is equivalent to the validity of equation (3.5). To establish the uniqueness result from (3.5), we introduce at present a simple lemma without proof.

Lemma 3.1. *Let $c_0\ne0$, $\mathbf{b}=[b_1,\cdots,b_{k-1}]^T$ be any solution of the equation $H_i(1,k-2,k-2)\mathbf{x}=0$. Then b_1 is identically equal to zero iff the matrix $H_i(1,k-2,k-2)$ is nonsingular.*

Theorem 3.1. *Suppose Padé approximation problem (1.1) has a solution; then it is unique if and only if one of the following three conditions is satisfied: 1) $c_0=0$ and $c_1^{(i)}=0,\quad i=1,\cdots,n$. 2) $c_0\ne0$ and $H_i(1,k-2,k-2)$ are nonsingular for $i=1,\cdots,n$. 3) $c_0\ne0$, there exists some l $(1\le l\le n)$ such that $H_l(1,k-2,k-2)$ is singular and*

$$\sum_{i=1}^{k}(-1)^{i-1}c_0^{k-i}\sum_{\substack{\alpha_1+\cdots+\alpha_i=\gamma\\ \alpha_j\ne0,j=1,\cdots,i}}c_{\alpha_1}\cdots c_{\alpha_i}=0,\quad |\gamma|=k.\tag{3.6}$$

Proof. 1) If $c_0 = 0$, then it follows from (3.5) that

$$\Delta = \sum_{\substack{\alpha+\beta=\gamma \\ \alpha\in N\setminus\{0\},\beta\in D\setminus\{0\}}} c_\alpha(b'_\beta - b_\beta) = 0, \quad |\gamma| = k+1. \tag{3.7}$$

From equation (2.2), we know that b_β can be any number for $\beta \in D$ and $|\beta| = k$. Hence (3.7) is valid if and only if $c_\alpha = 0$ for $|\alpha| = 1$.

2) Assume $c_0 \neq 0$. Rewrite (3.5) and (2.5) as

$$\Delta = \sum_{\substack{\alpha_2+\beta=\gamma \\ \alpha_2\in N\setminus\{0\},\beta\in D\setminus\{0\}}} [c_0(b_{\alpha_2}b'_\beta - b'_{\alpha_2}b_\beta) + c_{\alpha_2}(b'_\beta - b_\beta)] = 0, \quad |\gamma| = k+1. \tag{3.8}$$

Substituting (2.5) into (3.8), we have

$$\begin{aligned}\Delta = &- \sum_{\substack{\alpha_1+\alpha_2+\alpha_3=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\}, \\ \alpha_3\in D}} \{c_0c_0^{-1}[c_{\alpha_1}(b_{\alpha_2}b'_{\alpha_3} - b'_{\alpha_2}b_{\alpha_3})] + c_0^{-1}c_{\alpha_1}c_{\alpha_2}(b'_{\alpha_3} - b_{\alpha_3})\} \\ = &- \sum_{\substack{\alpha_1+\alpha_2=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\}}} c_{\alpha_1}(b_{\alpha_2} - b'_{\alpha_2}) \\ &- \sum_{\substack{\alpha_1+\alpha_2+\alpha_3=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\},\alpha_3\in D\setminus\{0\}}} \{c_0c_0^{-1}[c_{\alpha_1}(b_{\alpha_2}b'_{\alpha_3} - b'_{\alpha_2}b_{\alpha_3})] + c_0^{-1}c_{\alpha_1}c_{\alpha_2}(b'_{\alpha_3} - b_{\alpha_3})\}.\end{aligned}$$

It follows from (3.4) that

$$\begin{aligned}\Delta = &\sum_{\substack{\alpha_1+\alpha_2=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\}}} c_{\alpha_1}(b'_{\alpha_2} - b_{\alpha_2}) - \sum_{\substack{\alpha_1+\alpha_2+\alpha_3=\gamma \\ \alpha_1\neq 0,|\alpha_2|>1,\alpha_3\in D\setminus\{0\}}} c_0^{-1}c_{\alpha_1}c_{\alpha_2}(b'_{\alpha_3} - b_{\alpha_3}) \\ &- \sum_{\substack{\alpha_1+\alpha_2+\alpha_3=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\},\alpha_3\in D\setminus\{0\}}} c_0^{-1}c_{\alpha_1}c_{\alpha_2}(b'_{\alpha_3} - b_{\alpha_3}) \\ = &\sum_{\substack{\alpha_1+\alpha_2=\gamma \\ \alpha_1\neq 0,\alpha_2\in N\setminus\{0\}}} c_{\alpha_1}(b'_{\alpha_2} - b_{\alpha_2}) - \sum_{\substack{\alpha_1+\alpha_2+\alpha_3=\gamma \\ \alpha_1\neq 0,\alpha_2\neq 0,\alpha_3\in D\setminus\{0\}}} c_0^{-1}c_{\alpha_1}c_{\alpha_2}(b'_{\alpha_3} - b_{\alpha_3}).\end{aligned}$$

Using (2.5) repeatedly, we get at last

$$\Delta = \sum_{i=1}^{k}(-1)^{i-1}c_0^{-i+1} \sum_{\substack{\alpha_1+\cdots+\alpha_{i+1}=\gamma \\ \alpha_j\neq 0,j=1,\cdots,i \\ |\alpha_{i+1}|=1}} c_{\alpha_1}\cdots c_{\alpha_i}(b'_{\alpha_{i+1}} - b_{\alpha_{i+1}}), \quad |\gamma| = k+1.$$

Therefore the uniqueness is equivalent to

$$\sum_{i=1}^{k}(-1)^{i-1}c_0^{k-i} \sum_{\substack{\alpha_1+\cdots+\alpha_{i+1}=\gamma \\ \alpha_j\neq 0,j=1,\cdots,i,|\alpha_{i+1}|=1}} c_{\alpha_1}\cdots c_{\alpha_i}(b'_{\alpha_{i+1}} - b_{\alpha_{i+1}}) = 0, \quad |\gamma| = k+1. \tag{3.9}$$

If $H_i(1, k-2, k-2)$ are nonsingular for $i = 1, \cdots, n$, then $b'_\alpha - b_\alpha = 0$ for $|\alpha| = 1$. Hence (3.9) is valid.

3) If there exists some l such that $H_l(1, k-2, k-2)$ is singular, then from Lemma 3.1 we have that $b'_{e_l} - b_{e_l}$ can vary arbitrarily. Hence equality (3.9) is valid if and only if (3.6) is true. Then the theorem is proved.

Corollary 3.1. Let $k = 2$. Then Padé approximation problem (1.1) has unique solution if and only if one of the following three conditions is satisfied: 1) $c_0 = 0$ $c_1^{(i)} = 0$, $i = 1, \cdots, n$, and $c_2^{(i,j)} = 0$, $i, j = 1, \cdots, n$. 2) $c_0 \neq 0$ and $c_1^{(i)} \neq 0$, $i = 1, \cdots, n$. 3) $c_0 \neq 0$, there exists some l $(1 \leq l \leq n)$ such that $c_1^{(l)} = 0$ and

$$c_0 c_2^{(i,j)} = c_1^{(i)} c_1^{(j)}, \quad \forall i \neq j, \quad c_0 c_2^{(i)} = c_1^{(i)^2}, \quad i = 1, \cdots, n. \tag{3.10}$$

Proof. From Corollary 2.1 and Theorem 3.1, conclusions 1) and 2) are valid obviously. To prove 3), taking $\gamma = \mathbf{e}_i + \mathbf{e}_j$, $i \neq j$, then from (3.6) we get the first relation of (3.10). Taking $\gamma = 2\mathbf{e}_i$, then get the second relation. On the other hand, (3.10) implies (2.11).

§4. The Continuity of Padé Operator

From the definition of MPA and (2.1)–(2.2), MPA $p(\mathbf{x})/q(\mathbf{x})$ of $f(\mathbf{x}) = \sum_{\alpha \in \mathbf{Z}_+^n} c_\alpha \mathbf{x}^\alpha$ depends only on c_α with $|\alpha| \leq k$. Hence we may regard the operation of Padé approximation as a map from the space $\mathbf{R}^{|E|}$ into the space

$$\mathbf{R}(N, D) = \{R : R(\mathbf{x}) = \frac{\sum_{\alpha \in N} a_\alpha \mathbf{x}^\alpha}{\sum_{\beta \in D} b_\beta \mathbf{x}^\beta}, a_\alpha, b_\beta \in \mathbf{R},\ \mathbf{x} \in \mathbf{R}^n\},$$

i.e., we define the map P as follows

$$P : \mathbf{R}^{|E|} \longrightarrow \mathbf{R}(N, D) : Y \longmapsto R(\mathbf{x})$$

so that $P(Y)$ are the Padé approximants to $Y = [c_0, c_{e_1}, \cdots]^T \in \mathbf{R}^{|E|}$. P is referred to as Padé operator. From the discussion above, P may not be well defined and may have many values.

Let $Y \in \mathbf{R}^{|E|}$ be given and $P(Y) = p/q$ exist. If for any $\varepsilon > 0$ and any compact set D in $\mathbf{R}^n$ which does not contain the zeros of $q(\mathbf{x})$, there exists a $\delta > 0$ such that $\max_{\mathbf{x} \in D} |P(Y)(\mathbf{x}) - P(Y')(\mathbf{x})| < \varepsilon$ provided $\|Y - Y'\| < \delta$, then we say P is continuous at Y.

Suppose P is continuous at $Y \in \mathbf{R}^{|E|}$; then a) $P(Y)$ must exist. b) $P(Y)$ is unique. c) $P(Y)(x\mathbf{e}_i)$ are continuous as UPA operators for $i = 1, \cdots, n$.

Now we shall show that $c_0 \neq 0$. If $c_0 = 0$, from a) and b) we have $c_\alpha = 0$ for $\alpha \in E$, i.e., $Y = 0$. Let $Y' = [c_0, c_{e_1}, \cdots]^T \neq 0$ be given such that $c'_\alpha = 0$ *for* $|\alpha| \leq 1$, $\|Y - Y'\| < \delta$. Then by Theorem 2.1, $P(Y')$ does not exist. This contradicts the continuity of P. Therefore $c_0 \neq 0$. From the theory of UPA [13], we know that c) implies that $rank H_i(2, k-1, k-2) = k$, $i = 1, \cdots, n$. It follows from a), b) that $H_i(1, k-2, k-2)$ are nonsingular for $i = 1, \cdots, n$. Therefore we have had the necessary conditions for P to be continuous. Now we prove that the conditions obtained are also sufficient. Since $c_0 \neq 0$, and det $H_i(1, k-2, k-2) \neq 0$, there exists a $\delta > 0$ such that the same conclusions are true for Y' provided $\|Y' - Y\| < \delta$. Hence $P(Y') = p'/q'$ is well defined. From the continuity of UPA operator and relation (2.5), we have $p'(\mathbf{x}) \longrightarrow p(\mathbf{x})$, $q'(\mathbf{x}) \longrightarrow q(\mathbf{x})$, *as* $Y' \longrightarrow Y$. Therefore the continuity is valid. Hence we have

Theorem 4.1. *Padé operator P is continuous at Y if and only if $c_0 \neq 0$, and $H_i(1, k-2, k-2)$ are nonsingular for $i = 1, \cdots, n$.*

§5. Application

Let $F(\mathbf{x}) = [f_1(\mathbf{x}), f_2(\mathbf{x}) \cdots f_n(\mathbf{x})]^T, \mathbf{x} \in \mathbf{R}^n$. We now use Padé approximants of $f_i(\mathbf{x})$ to construct an iterative process for finding zeros of F. Let $\mathbf{x}^* \in \mathbf{R}^n$ be a zero of F, i.e.,

$F(\mathbf{x}^*)=0$, $\mathbf{x}^{(0)}$ be a starting value and $p_i(\mathbf{x}^{(k)},\mathbf{x})/q_i(\mathbf{x}^{(k)},\mathbf{x})$ be the Padé approximants of $f_i(\mathbf{x})$ at $\mathbf{x}^{(k)}$ for $k\geq 0$. Then $\mathbf{x}^{(k+1)}$ is determined successively by

$$p_i(\mathbf{x}^{(k)},\mathbf{x}^{(k+1)})=0,\quad i=1,\cdots,n. \tag{5.1}$$

Since $p_i(\mathbf{x}^{(k)},\mathbf{x})=f_i(\mathbf{x}^{(k)})+\sum_{j=1}^{n}a_j^{(i)}(\mathbf{x}^{(k)})(x_j-x_j^{(k)})$, we have from (5.1)

$$\mathbf{x}^{(k+1)}=\mathbf{x}^{(k)}-A^{-1}(\mathbf{x}^{(k)})F(\mathbf{x}^{(k)}),\quad k=0,1,\cdots, \tag{5.2}$$

where $A(\mathbf{x}^{(k)})=(a_j^{(i)}(\mathbf{x}^{(k)}))_{i,j=1}^{n}$. Suppose Padé operator P is continuous at f_i; then all $a_j^{(i)}(\mathbf{x}^{(k)})$ are well defined. They can be evaluated recursively by Baker's algorithm. We recall that the specific formulas for $k=2,3,4$ are given in §2. Let

$$H_j(f_i,\mathbf{x},1,k-2,k-2)=\begin{bmatrix} D_jf_i(\mathbf{x}) & f_i(\mathbf{x}) & & & \\ D_j^2f_i(\mathbf{x})/2! & D_jf_i(\mathbf{x}) & f_i(\mathbf{x}) & & \\ \vdots & \vdots & \vdots & \ddots & \\ D_j^{k-1}f_i(\mathbf{x})/(k-1)! & D_j^{k-2}f_i(\mathbf{x})/(k-2)! & D_j^{k-3}f_i(\mathbf{x})/(k-3)! & \cdots & f_i(\mathbf{x}) \end{bmatrix}.$$

Then $a_j^{(i)}(\mathbf{x}^{(k)})$ can be expressed explicitly as

$$a_j^{(i)}(\mathbf{x}^{(k)})=D_jf_i(\mathbf{x}^{(k)})-\frac{f_i(\mathbf{x}^{(k)})}{\det H_j(f_i,\mathbf{x}^{(k)},1,k-2,k-2)}$$

$$\times\det\begin{bmatrix} D_j^2f_i(\mathbf{x}^{(k)})/2! & f_i(\mathbf{x}^{(k)}) & & & \\ D_j^3f_i(\mathbf{x}^{(k)})/3! & D_jf_i(\mathbf{x}^{(k)}) & f_i(\mathbf{x}^{(k)}) & & \\ \vdots & \vdots & \vdots & \ddots & \\ D_j^kf_i(\mathbf{x}^{(k)})/(k)! & D_j^{k-2}f_i(\mathbf{x}^{(k)})/(k-2)! & D_j^{k-3}f^i(\mathbf{x}^{(k)})/(k-3)! & \cdots & f_i(\mathbf{x}^{(k)}) \end{bmatrix}.$$

Hence $A(\mathbf{x}^{(k)})$ can be rewritten as $A(\mathbf{x}^{(k)})=DF(\mathbf{x}^{(k)})-diag(f_1(\mathbf{x}^{(k)}),\cdots,f_n(\mathbf{x}^{(k)}))B(\mathbf{x}^{(k)})$, where $DF(\mathbf{x})$ is the Fréchet–derivative of F. Under some conditions on F,

$$A(\mathbf{x})\longrightarrow DF(\mathbf{x}^*)\quad\text{as}\quad \mathbf{x}\longrightarrow\mathbf{x}^*. \tag{5.3}$$

Therefore (5.2) is a kind of modified Newton method (see [11],[12]) .

Theorem 5.1. *Let $C_0\subset\mathbf{R}^n$ be an open set. Let $f_i(\mathbf{x})$ be continuous on C_0 and have required partial derivatives such that* $\det H_i(f_j,\mathbf{x},1,k-2,k-2)\neq 0$ *for $i,j=1,\cdots,n$, $\mathbf{x}\in C_0$, and $|a_j^{(i)}(\mathbf{x})|$ are bounded above in C_0.*

For $\mathbf{x}^{(0)}\in C_0$ let positive constants r,α,β,γ,h and integer m be given with the following properties:

$$S_r(\mathbf{x}^{(0)})=\{\mathbf{x}:\|\mathbf{x}-\mathbf{x}^{(0)}\|<r\}\subset C_0,\quad r=\alpha/(1-h),\quad h=\alpha^{\frac{1}{m}}(\beta\gamma)^{\frac{1}{mm}}<1,$$

and let $F(\mathbf{x})$ have the properties

(a) $|f_i(\mathbf{x})-p_i(\mathbf{y},\mathbf{x})/q_i(\mathbf{y},\mathbf{x})|\leq\gamma\|\mathbf{x}-\mathbf{y}\|^{m+1}$, for all $\mathbf{x},\mathbf{y}\in C_0$, and $i=1,\cdots,n$.

(b) $A^{-1}(\mathbf{x})$ exists and satisfies $\|A^{-1}(\mathbf{x})\|\leq\beta$ for all $\mathbf{x}\in C_0$.

(c) $\|A^{-1}(\mathbf{x}^{(0)})F(\mathbf{x}^{(0)})\|\leq\alpha$. Then 1) Beginning at $\mathbf{x}^{(0)}$, the sequence $\{\mathbf{x}^{(k)}\}$ generated by (5.2) is well defined and $\mathbf{x}^{(k)}\in S_r(\mathbf{x}^{(0)})$ for all $k\geq 0$. 2) $\lim_{k\to\infty}\mathbf{x}^{(k)}=\mathbf{x}^*$ exists, and $\mathbf{x}^*\in\overline{S_r(\mathbf{x}^{(0)})}$ and $F(\mathbf{x}^*)=0$. 3) For all $k\geq 0$. $\|\mathbf{x}^{(k)}-\mathbf{x}^*\|\leq\alpha\frac{h^{(m+1)^k-m}}{1-(h^{(m+1)^k})^m}$. Since $0<h<1$, Padé method (5.2) is convergent with order at least $m+1$.

Proof. 1) Since $A^{-1}(\mathbf{x})$ exists for $\mathbf{x} \in C_0$, $\mathbf{x}^{(k+1)}$ is well defined for all k if $\mathbf{x}^{(k)} \in S_r(\mathbf{x}^{(0)})$ for all $k \geq 0$. This is valid for $k = 0$ and $k = 1$ by assumption (c). Now, if $\mathbf{x}^{(j)} \in S_r(\mathbf{x}^{(0)})$ for $j = 0, 1, \cdots, k$, then from assumption (b),

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\| = \| - A^{-1}(\mathbf{x}^{(k)})F(\mathbf{x}^{(k)})\| \leq \beta\|F(\mathbf{x}^{(k)}\| \leq \beta \max_{1\leq i\leq n} |f_i(\mathbf{x}^{(k)}) - p_i(\mathbf{x}^{(k-1)}, \mathbf{x}^{(k)})/q_i(\mathbf{x}^{(k-1)}, \mathbf{x}^{(k)})| \leq \gamma\beta\|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|^{m+1}. \tag{5.4}$$

From this we have by induction

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\| \leq \alpha h^{(m+1)^k - m}. \tag{5.5}$$

Hence

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(0)}\| \leq \|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\| + \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\| + \cdots + \|\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\| \leq \alpha(1 + h + h^{(m+1)^2 - m} + \cdots + h^{(m+1)^k - m}) < \alpha/(1-h) = r$$

and consequently $\mathbf{x}^{(k+1)} \in S_r(\mathbf{x}^{(0)})$.

2) From (5.5) it is easily determined that $\{\mathbf{x}^{(k)}\}$ is a Cauchy sequence, since for $k \geq t$ we have

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(t)}\| \leq \alpha h^{(m+1)^t - m}[1 + (h^{(m+1)^t})^m + (h^{(m+1)^t})^{(m+1)^2 - 1} + \cdots] < \alpha \frac{h^{(m+1)^t - m}}{1 - (h^{(m+1)^t})^m} < \varepsilon \tag{5.6}$$

for sufficiently large $t \geq N(\varepsilon)$, because $0 < h < 1$. Consequently, there is a limit $\lim_{k\to\infty} \mathbf{x}^{(k)} = \mathbf{x}^* \in \overline{S_r(\mathbf{x}^{(0)})}$. By passing to the limit as $k \to \infty$ in (5.6) we obtain 3). We must still show that $\mathbf{x}^*$ is a zero of F in $\overline{S_r(\mathbf{x}^{(0)})}$. Since the elements of $A(\mathbf{x})$ are bounded on C_0, $\|A(\mathbf{x})\|$ is bounded above in $\overline{S_r(\mathbf{x}^{(0)})}$. It follows from (5.2) that $\|F(\mathbf{x}^{(k)})\| \leq \|A(\mathbf{x}^{(k)})\|\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\|$. Hence $\lim_{k\to\infty} \|F(\mathbf{x}^{(k)})\| = 0$. Since F is continuous at $\mathbf{x}^*$, $\lim_{k\to\infty} \|F(\mathbf{x}^{(k)})\| = \|F(\mathbf{x}^*)\| = 0$.

Theorem 5.1 characterizes the starting value $\mathbf{x}^{(0)}$, such that beginning at $\mathbf{x}^{(0)}$, the sequence $\{\mathbf{x}^{(k)}\}$ generated by (5.2) is convergent to a zero $\mathbf{x}^*$ of F. Now we give a result which characterizes the limit $\mathbf{x}^*$ for the convergence.

Corollary 5.1. Let $\mathbf{x}^*$ be given. $F(\mathbf{x})$ have the following properties: (a) $F(\mathbf{x})$ is continuous in $S_r(\mathbf{x}^*)$, a neighbourhood of $\mathbf{x}^*$. (b) $F(\mathbf{x}^*) = 0$, $F(\mathbf{x}) \neq 0$, for $\mathbf{x} \in S_r(\mathbf{x}^*)\backslash\{\mathbf{x}^*\}$. (c) F has Fréchet derivative $DF(\mathbf{x}^*)$ and $DF(\mathbf{x}^*)$ is nonsingular. (d) $detH_i(f_j, \mathbf{x}, 1, k-2, k-2) \neq 0$ *for* $i, j = 1, \cdots, n$, $\mathbf{x} \in S_r(\mathbf{x}^*)$, and $|a_j^{(i)}(\mathbf{x})|$ are continuous at $\mathbf{x}^*$. (e) $\|F(\mathbf{x}) - p(\mathbf{y}, \mathbf{x})/q(\mathbf{y}, \mathbf{x})\| \leq \gamma\|\mathbf{x} - \mathbf{y}\|^{m+1}$, for all $\mathbf{x}, \mathbf{y} \in S_r(\mathbf{x}^*)$. Then

1) If $\mathbf{x}^{(0)}$ is close enough to $\mathbf{x}^*$, the sequence $\{\mathbf{x}^{(k)}\}$ generated by (5.2) is well defined.

2) $\lim_{k\to\infty} \mathbf{x}^{(k)} = \mathbf{x}^*$. 3) If $\mathbf{x}^{(k)} \neq \mathbf{x}^*$ for $k \geq k_0$, then there exist constants C and k_1 such that

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\| \leq C\|\mathbf{x}^{(k)} - \mathbf{x}^*\|^{m+1}, \quad \text{for } k \geq k_1.$$

Proof. Under the assumptions of the corollary, (5.3) holds. Then $A^{-1}(\mathbf{x}^*)$ exists. From the perturbation lemma for matrices (see [11], p.7) we have that $A(\mathbf{x})$ is nonsingular and $\|A^{-1}(\mathbf{x})\| \leq \beta$, *for* $\mathbf{x} \in S_{r_1}(\mathbf{x}^*)$ $\beta > \|A^{-1}(\mathbf{x}^*)\|$, and $r_1 \leq r$. Therefore, for $C_0 = S_{r_1}(\mathbf{x}^*)$, the conditions of Theorem 5.1 are satisfied for a certain set of constants $r, \alpha, \beta, \gamma, h$ and a suitable $\mathbf{x}^{(0)}$. Then the conclusions 1) and 2) are valid from Theorem 5.1. Now we prove 3). Let $\varepsilon > 0$ be given. Then there exists a $\delta > 0$ under the assumptions of the corollary, such that for $\mathbf{x} \in S_\delta(\mathbf{x}^*)$ $\|F(\mathbf{x}) - F(\mathbf{x}^*) - DF(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*)\| \leq \frac{\varepsilon}{2\beta}\|\mathbf{x} - \mathbf{x}^*\|$, $\|A^{-1}(\mathbf{x})A(\mathbf{x}^*) - I\| \leq \frac{\varepsilon}{2}$.

Then

$$\|-A^{-1}(\mathbf{x})F(\mathbf{x})+\mathbf{x}-\mathbf{x}^*\| \le \|A^{-1}(\mathbf{x})[F(\mathbf{x})-DF(\mathbf{x}^*)(\mathbf{x}-\mathbf{x}^*)]\| + \|[A^{-1}(\mathbf{x})A(\mathbf{x}^*)-I](\mathbf{x}-\mathbf{x}^*)\| \le \varepsilon\|\mathbf{x}-\mathbf{x}^*\|.$$

It follows that $\lim_{\mathbf{x}\to\mathbf{x}^*} \frac{\|-A^{-1}(\mathbf{x})F(\mathbf{x})+\mathbf{x}-\mathbf{x}^*\|}{\|\mathbf{x}-\mathbf{x}^*\|} = 0$. Hence if $\mathbf{x}^{(k)} \ne \mathbf{x}^*$,

$$\lim_{k\to\infty} \frac{\|\mathbf{x}^{(k+1)}-\mathbf{x}^*\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|} = \lim_{k\to\infty} \frac{\|-A^{-1}(\mathbf{x}^{(k)})F(\mathbf{x}^{(k)})+\mathbf{x}^{(k)}-\mathbf{x}^*\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|} = 0.$$

Since

$$\left|\frac{\|\mathbf{x}^{(k+1)}-\mathbf{x}^{(k)}\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|} - \frac{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|}\right| \le \frac{\|\mathbf{x}^{(k+1)}-\mathbf{x}^*\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|}, \quad \lim_{k\to\infty} \frac{\|\mathbf{x}^{(k+1)}-\mathbf{x}^{(k)}\|}{\|\mathbf{x}^{(k)}-\mathbf{x}^*\|} = 1.$$

Therefore, there exist $\sigma_1 < 1$, $\sigma_2 > 1$ and $k_1 \ge k_0$, such that $\sigma_1\|\mathbf{x}^{(k)}-\mathbf{x}^*\| \le \|\mathbf{x}^{(k+1)}-\mathbf{x}^{(k)}\| \le \sigma_2\|\mathbf{x}^{(k)}-\mathbf{x}^*\|$, for $k \ge k_1$. From (5.8) it follows that

$$\|\mathbf{x}^{(k+1)}-\mathbf{x}^*\| \le \sigma_1^{-1}\|\mathbf{x}^{(k+2)}-\mathbf{x}^{(k+1)}\| \le \gamma\beta\sigma_1^{-1}\|\mathbf{x}^{(k+1)}-\mathbf{x}^{(k)}\|^{m+1} \le \gamma\beta\sigma_1^{-1}\sigma_2^{m+1}\|\mathbf{x}^{(k)}-\mathbf{x}^*\|^{m+1} = C|\mathbf{x}^{(k)}-\mathbf{x}^*\|^{m+1}.$$

Then 3) is proved.

Table 5.1

Starting Values	Newton	(5.2)	Starting Values	Newton	(5.2)
(5.3, 0.3)	29	5	(3.4, 1.4)	15	4
(4.3, 0.2)	12	4	(3.6, 1.6)	20	5
(1.0, −1.0)	7	4	(4.0, 2.0)	42	5
(3.0, 1.0)	9	4	(4.4, 2.4)	90	5
(3.2, 1.2)	11	4	(4.8, 2.8)	200	6

Table 5.2

Starting Values	Newton	(5.2)	Starting Values	Newton	(5.2)
$-1.0x^*$	overflow	13	$0.9x^*$	7	4
$0.0x^*$	overflow	10	$1.4x^*$	8	5
$0.6x^*$	overflow	6	$1.8x^*$	13	8
$0.63x^*$	109	6	$2.3x^*$	20	11
$0.7x^*$	38	6	$2.7x^*$	25	14

Remark 1. According to the definition of MPA, m in condition (a) of Theorem 5.1 or condition (e) of Corollary 5.1 can be taken as k defined in (1.3)–(1.4). Hence a higher order iterative scheme may be achieved by taking k larger. The cost is to compute high order derivatives of F. For $k = 2$, $D_j f_i(\mathbf{x}^{(k)})$ and $D_j^2 f_i(\mathbf{x}^{(k)})$ are needed. They can be replaced by the first and second order differences of $f_i(\mathbf{x}^{(k)})$ in the direction $\mathbf{e}_j$ if the derivatives are difficult to evaluate. It should be pointed out that iterative scheme (5.2) does not relate to the mixed partial derivatives. This is an advantage of our method compare with other the same order methods, such as Chebyshev method ([5],p.100), Halley method, and tangent hyperbolas method.

2. Similarly to Newton method, the convergence of (5.2) can be guaranteed only in some small neighborhood of $\mathbf{x}^*$. However, in some cases, the convergence range of (5.2) is

larger than that of Newton method. The following example, in which $\|\mathbf{x}^{(h)} - \mathbf{x}^*\| \le 10^{-15}$, will do the illastration.

Example 5.1. Let $n = 2$, $k = 2$, $F(\mathbf{x}) = [\exp(-x_1 + x_2) - 0.1 \exp(-x_1 - x_2) - 0.1]^T$. $F(\mathbf{x})$ has a simple zero $\mathbf{x}^* = [-ln(0.1),\ 0]^T$. The iterative times required for different starting values are listed in Table 5.1.

Example 5.2. Let $n = 12$, $k = 2$, $F(\mathbf{x}) = [g_1(\mathbf{x}) - g_1(1), \cdots, g_n(\mathbf{x}) - g_n(1)]^T$, where $g_i(\mathbf{x}) = \exp(A_i\mathbf{x}) + 0.2\sin(B_i\mathbf{x}) + 0.1\cos(C_i\mathbf{x})$, $A_i = (T_{i-1}(t_j))_{j=1}^n$, $B_i = ((\frac{i}{n})^{j-1})_{j=1}^n$, $C_i = (\frac{1}{i+j-1})_{j=1}^n$, for $i = 1, \cdots, n$ and T_n is the Chebyshev polynomial of degree n , $t_i = \cos\frac{(i-1)\pi}{n-1}$. $F(\mathbf{x})$ has a simple zero $\mathbf{x}^* = [1, \cdots, 1]^T$. The computing results are given in Table 5.2.

From the examples given above, we can see that for some functions Padé approximation method (5.2) has not only larger convergence range, but also faster convergence rate compared with Newton method. Of course, method (5.2) can not always behave so well for all functions. The next example will do the illustration.

Example 5.3. Let $n = 5$, $k = 2$, $g_i(\mathbf{x}) = \exp(A_i\mathbf{x}) + 0.2\sin(B_i\mathbf{x}) + 0.1\cos(C_i\mathbf{x})$ $f_i(\mathbf{x}) = g_i(\mathbf{x}) - g_i(1)$, $i = 1, \cdots, n$, where $A_i = (\frac{1}{i+j-1})_{j=1}^n$, $B_i = ((\frac{i}{n})^{j-1})_{j=1}^n$, $C_i = (T_{i-1}(t_j))_{j=1}^n$. $F(\mathbf{x}) = [f_1(\mathbf{x}), \cdots, f_n(\mathbf{x})]^T$ has a simple zero $\mathbf{x}^* = [1, \cdots, 1]^T$. The computing results are shown in Table 5.3.

Table 5.3

Starting Values	Newton	(5.2)	Starting Values	Newton	(5.2)
$0.85x^*$	failure	failure	$1.3x^*$	9	9
$0.9x^*$	8	6	$1.4x^*$	failure	failure

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