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On a one-dimensional optimization problem derived from the efficiency analysis of Newton-PCG-like algorithms ☆

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Abstract

The Newton-PCG (preconditioned conjugate gradient) like algorithms are usually very efficient. However, their efficiency is mainly supported by the numerical experiments. Recently, a new kind of Newton-PCG-like algorithms is derived in (J. Optim. Theory Appl. 105 (2000) 97; Superiority analysis on truncated Newton method with preconditioned conjugate gradient technique for optimization, in preparation) by the efficiency analysis. It is proved from the theoretical point of view that their efficiency is superior to that of Newton's method for the special cases where Newton's method converges with precise Q-order 2 and $\alpha(\geqslant 2)$, respectively. In the process of extending such kind of algorithms to the more general case where Newton's method has no fixed convergence order, the first is to get the solutions to the one-dimensional optimization problems with many different parameter values of α. If these problems were solved by numerical method one by one, the computation cost would reduce the efficiency of the Newton-PCG algorithm, and therefore is unacceptable. In this paper, we overcome the difficulty by deriving an analytic expression of the solution to the one-dimensional optimization problem with respect to the parameter α.

MSC: 65K05; 90C30

Keywords: Newton-PCG-like algorithm; One-dimensional optimization problem; Analytic expression

1. Introduction

For the unconstrained optimization problem

$$\min f(x), \quad x \in R^n \tag{1.1}$$

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Newton's method is a basic method. The study on improving it has been continued for many years. The Newton-PCG (preconditioned conjugate gradient) like algorithms are one kind of the improved methods. It has been shown that they are usually very efficient (see e.g. [1,3–5]). However, their efficiency is mainly supported by the numerical experiments.

Recently, a new kind of Newton-PCG-like algorithms is derived in [2,7] from some algorithm models by an efficiency analysis. It is proved from the theoretical point of view that their efficiency is superior to that of Newton's method. The basic idea to construct the algorithms model is that the Newton equations are solved exactly by Cholesky factorization (CF step) or approximately by preconditioned conjugate gradient method (PCG step). More precisely, the models are made up by circles. Each circle consists of one CF step and p PCG steps, where p is a parameter. The key point is to choose such p in the model that the efficiency (or its approximation) of the algorithms to be maximized. In detail, in each circle, the CF step is executed firstly, and the value of p is obtained by solving a one-dimensional optimization problem which is established according to the progress speed of the CF step, then p PCG steps are executed.

In fact, [2] is concerned with the case where the Newton's method is precisely quadratically convergent. In this case, the progress speed of CF step in every circle is "the same". Therefore, there is only *one* one-dimensional optimization problem to be solved and the computation cost is negligible. In [7] the corresponding convergence Q-order is assumed to be a fixed scalar $\alpha(\geqslant 2)$ but unknown. So in each circle, the progress speed of CF step, say α_k, is calculated firstly, then a one-dimensional optimization problem established according to α_k should be solved. However, noticing that

$$\alpha_k \to \alpha, \tag{1.2}$$

eventually, there are at most two one-dimensional optimization problems to be solved. Therefore, the computation cost is still acceptable.

This paper deals with the more general case where the convergence speed of Newton's method is unknown and even Newton's method may have no a fixed convergence order. We assume that the convergence speed of Newton's method is allowed to be in some interval, say $[\alpha_l, \alpha_h]$, in the following sense: There exist $\delta > 0$, $M_l \geqslant M_h > 0$, α_l and α_h such that when $\|x_c - x^*\| < \delta$ (x^* is the solution of (1.1))

$$M_h\|x_c - x^*\|^{\alpha_h} \leqslant \|x_+ - x^*\| \leqslant M_l\|x_c - x^*\|^{\alpha_l}, \tag{1.3}$$

where

$$x_+ \overset{\text{def}}{=} x_c - \nabla^2 f(x_c)^{-1}\nabla f(x_c). \tag{1.4}$$

In this case, the convergence speed of Newton's method is not a fixed number any more. Therefore, in a circle of the new Newton-PCG-like algorithm, we first calculate the approximate progress speed of CF step, say α_k, $k=1,2,\ldots$, and establish the corresponding one-dimensional optimization problem, then take the solution as p to finish the following PCG steps of this circle. Noting that instead of the validity of (1.2), these α_k may be any points in the interval $[\alpha_l, \alpha_h]$. So we have to solve a series of the one-dimensional optimization problems instead of the two ones in [7]. If these problems were solved by numerical method one by one, the computation cost would reduce the efficiency of the new Newton-PCG algorithm dramatically, and therefore, is unacceptable. This is the first difficulty for us to establish the new algorithm.

In this paper, the above difficulty is overcome by deriving an *analytic* expression of the solution to the one-dimensional optimization problem with the parameter α.

The paper is organized as follows: Section 2 gives some lemmas, which are used to derive the analytic expression of the solution (Theorem 3.1) in Section 3.

2. Some lemmas

Extending the Newton-PCG algorithms in [2,7] leads to the one-dimensional problem with a parameter α:

$$P(n,\alpha)\colon \min_K u(K;n,\alpha) = \frac{1+\sum_{m=1}^{K}\varphi(\alpha,m)Q(n)}{1+K}, \tag{2.1}$$

$$\text{s.t.} \quad K \text{ is a nonnegative integer}, \tag{2.2}$$

where n is the dimension of the optimization problem (1.1), $\varphi(\tau,q)$ is an integer function satisfying

$$(\tau)^q(\tau-1) < \varphi(\tau,q) \leqslant (\tau)^q(\tau-1)+1 \tag{2.3}$$

and

$$Q(n) = (2n^2+6n+2)/(n^3/6+3n^2/2-2n/3). \tag{2.4}$$

(Note that when $K=0$, we define the "sum" $\sum_{m=1}^{K}\cdots = 0$.)

In fact, for a certain circle in the new algorithm model, α is the calculating value of the progress speed of CF step and the solution $K^* = K^*(n,\alpha)$ to problem (2.1)–(2.4) is taken as the PCG step number, i.e. the value of p. Just as mentioned above, in different circles, the values of α can be different in $[\alpha_l,\alpha_h]$. So, we will have a series of different one-dimensional problems in different circle. The cost of solving them is not negligible. This difficulty can be overcome by obtaining the analytic expression with respect to the parameter α for this solution, and the value of p in each circle can be obtained easily by the analytic expression. Theorem 3.1 in Section 3 will give this analytic expression. To derive Theorem 3.1, we give five lemmas in this section.

Lemma 2.1. *For $\alpha \geqslant 2$, $K^* = K^*(n,\alpha)$ is the smallest global solution to the problem $P(n,\alpha)$ defined by* (2.1)–(2.4) *if and only if*

$$u(0;n,\alpha) > u(1;n,\alpha) > \cdots > u(K^*;n,\alpha) \leqslant u(K^*+1;n,\alpha) < u(K^*+2;n,\alpha) < \cdots. \tag{2.5}$$

Proof. If (2.5) is valid, K^* is obviously the smallest global solution to the problem $P(n,\alpha)$. Now we prove that (2.5) is valid when K^* is the smallest global solution to the problem $P(n,\alpha)$ by the following three steps.

(1) we prove the following conclusion: if

$$u(\tilde{K};n,\alpha) \leqslant u(\tilde{K}+1;n,\alpha), \tag{2.6}$$

then

$$u(\tilde{K}+1;n,\alpha) < u(\tilde{K}+2;n,\alpha) \tag{2.7}$$

for all positive integer $\tilde{K}$. In fact, when $\alpha \geqslant 2$, we have

$$(\alpha)^1(\alpha-1) < (\alpha)^2(\alpha-1) < \cdots,$$

$$(\alpha)^1(\alpha-1)+1 < (\alpha)^2(\alpha-1)+1 < \cdots.$$

Therefore, by definition (2.3) of φ, the sequence $\{\varphi(\alpha,m)Q(n)\}$ is increasing

$$\varphi(\alpha,1)Q(n) < \varphi(\alpha,2)Q(n) < \cdots. \tag{2.8}$$

Since $u(\tilde{K}+1;n,\alpha)$ can be written as

$$u(\tilde{K}+1;n,\alpha) = \frac{(1+\tilde{K})u(\tilde{K};n,\alpha)+\varphi(\alpha,\tilde{K}+1)Q(n)}{1+(\tilde{K}+1)} \tag{2.9}$$

it is shown by (2.6) that

$$u(\tilde{K};n,\alpha) \leqslant \varphi(\alpha,\tilde{K}+1)Q(n). \tag{2.10}$$

Therefore, by (2.9)

$$u(\tilde{K}+1;n,\alpha) \leqslant \varphi(\alpha,\tilde{K}+1)Q(n). \tag{2.11}$$

On the other hand, $u(\tilde{K}+2;n,\alpha)$ can be written as

$$u(\tilde{K}+2;n,\alpha) = \frac{(1+\tilde{K}+1)u(\tilde{K}+1;n,\alpha)+\varphi(\alpha,\tilde{K}+2)Q(n)}{1+(\tilde{K}+2)}.$$

So by (2.8) and (2.11), we have

$$u(\tilde{K}+2;n,\alpha) > \frac{(1+\tilde{K}+1)u(\tilde{K}+1;n,\alpha)+u(\tilde{K}+1;n,\alpha)}{1+(\tilde{K}+2)} = u(\tilde{K}+1;n,\alpha).$$

The proof of (2.7) is completed.

(2) we prove the following conclusion: if

$$u(\tilde{K}-1;n,\alpha) > u(\tilde{K};n,\alpha), \tag{2.12}$$

then

$$u(\tilde{K}-2;n,\alpha) > u(\tilde{K}-1;n,\alpha) \tag{2.13}$$

for any integer $\tilde{K} \geqslant 2$. In fact, by (2.12) and definition (2.1) of u, we have

$$1+\sum_{m=1}^{\tilde{K}-2}\varphi(\alpha,m)Q(n) > \tilde{K}\varphi(\alpha,\tilde{K})Q(n)-\varphi(\alpha,\tilde{K}-1)Q(n). \tag{2.14}$$

In order to prove (2.13), by definition (2.1) of u again, we only need to prove

$$1+\sum_{m=1}^{\tilde{K}-2}\varphi(\alpha,m)Q(n) > (\tilde{K}-1)\varphi(\alpha,\tilde{K}-1)Q(n). \tag{2.15}$$

So by (2.14), we only need to prove

$$\tilde{K}\varphi(\alpha,\tilde{K})Q(n) - \varphi(\alpha,\tilde{K}-1)Q(n) > (\tilde{K}-1)\varphi(\alpha,\tilde{K}-1)Q(n)$$

or

$$\tilde{K}[\varphi(\alpha,\tilde{K}) - \varphi(\alpha,\tilde{K}-1)]Q(n) > 0. \tag{2.16}$$

However, by (2.8) and (2.16) is valid. Therefore, (2.13) is proved.

(3) we prove (2.5) for the smallest global solution K^*. Reminding the validity of (2.7), $u(K^*-1;n,\alpha) \leqslant u(K^*;n,\alpha)$ implies that K^* is not the smallest global solution to $P(n,\alpha)$. Therefore, we have

$$u(K^*-1;n,\alpha) > u(K^*;n,\alpha). \tag{2.17}$$

On the other hand, we have

$$u(K^*;n,\alpha) \leqslant u(K^*+1;n,\alpha). \tag{2.18}$$

Therefore, (2.5) follows from (2.17), (2.18), (2.7) and (2.13). □

Due to Lemma 2.1, in order to solve the problem $P(n,\alpha)$, we only need to examine the sequence $u(0;n,\alpha)$, $u(1;n,\alpha),\ldots$ until it becomes increasing.

Lemma 2.2. *For the problem $P(n,\alpha)$, both the objective function $u(K;n,\alpha)$ and its smallest global solution $K^*(n,\alpha)$ are right-continuous functions with respect to α.*

Proof. The results are obtained by the fact that $\varphi(\alpha,m)$ is a right-continuous function with respect to α. □

Lemma 2.3. *The smallest global solution $K^*(n,\alpha)$ of the problem $P(n,\alpha)$ is nonincreasing with respect to α when $\alpha \geqslant 2$.*

Proof. We first prove that for any $\alpha_2 > 2$, there exists $\delta > 0$ such that

$$K_2^* \leqslant K_1^* \quad \text{for } \alpha_1 \in (\alpha_2-\delta,\alpha_2), \tag{2.19}$$

where $K_2^* = K^*(n,\alpha_2)$ and $K_1^* = K^*(n,\alpha_1)$. We, respectively, prove (2.19) for the two cases

$$K_1^* = 0 \tag{2.20}$$

and

$$K_1^* \geqslant 1. \tag{2.21}$$

For case (2.20), i.e. $K_1^* = 0$, it is sufficient to show $K_2^* = 0$. In fact, since $K_1^* = 0$, we have

$$1 \leqslant u(1;n,\alpha_1). \tag{2.22}$$

However, by definition (2.3) of φ, for $\alpha_1 < \alpha_2$, we have

$$\varphi(\alpha_1,1) \leqslant \varphi(\alpha_2,1). \tag{2.23}$$

Therefore,

$$u(1;n,\alpha_1) \leqslant u(1;n,\alpha_2). \tag{2.24}$$

By (2.22) and (2.24) and Lemma 2.1, we know that $K_2^* = 0$. So (2.19) is proved.

For case (2.21), by definition (2.3) of φ, we see that, for $m = 1,2,\ldots,K_1^*+1$

$$\lim_{\eta\to+0}\varphi(\alpha_2-\eta,m) = \begin{cases} \varphi(\alpha_2,m)-1 & \text{if } \alpha_2 \text{ is an integer,} \\ \varphi(\alpha_2,m) & \text{otherwise.} \end{cases}$$

Therefore, noticing φ is an integer function, we conclude that there exist $\eta_m > 0$ $(m=1,2,\ldots,K_1^*+1)$ such that when $0 < \eta < \eta_m$

$$\varphi(\alpha_2-\eta,m) = \begin{cases} \varphi(\alpha_2,m)-1 & \text{if } \alpha_2 \text{ is an integer,} \\ \varphi(\alpha_2,m) & \text{otherwise.} \end{cases} \tag{2.25}$$

Defining

$$\delta = \min\{\eta_m \mid m = 1,2,\ldots,K_1^*+1\} \tag{2.26}$$

equality (2.25) leads to that for any $\alpha_1 \in (\alpha_2-\delta,\alpha_2)$

$$\varphi(\alpha_2,m) - \varphi(\alpha_1,m) = \begin{cases} 1 \text{ if } \alpha_2 \text{ is an integer,} \\ 0 \text{ otherwise.} \end{cases} \tag{2.27}$$

Therefore, by definition (2.1) of u

$$\begin{aligned} u(K_1^*;n,\alpha_2) - u(K_1^*;n,\alpha_1) &= \frac{\sum_{m=1}^{K_1^*}[\varphi(\alpha_2,m)-\varphi(\alpha_1,m)]Q(n)}{1+K_1^*} \\ &\leqslant [\varphi(\alpha_2,K_1^*+1)-\varphi(\alpha_1,K_1^*+1)]Q(n). \end{aligned}$$

The above inequality can be rewritten as

$$\varphi(\alpha_1,K_1^*+1)Q(n) - u(K_1^*;n,\alpha_1) \leqslant \varphi(\alpha_2,K_1^*+1)Q(n) - u(K_1^*;n,\alpha_2). \tag{2.28}$$

Since K_1^* is the smallest global solution to the problem $P(n,\alpha_1)$ defined by (2.1)–(2.4) with α there being replaced by α_1, by Lemma 2.1, we have

$$u(K_1^*;n,\alpha_1) \leqslant u(K_1^*+1;n,\alpha_1). \tag{2.29}$$

So by (2.29) and (2.11) with $\tilde{K}$ there being replace d by K_1^*

$$u(K_1^*;n,\alpha_1) \leqslant \varphi(\alpha_1,K_1^*+1)Q(n). \tag{2.30}$$

Combining (2.28) and (2.30) yields

$$u(K_1^*;n,\alpha_2) \leqslant \varphi(\alpha_2,K_1^*+1)Q(n). \tag{2.31}$$

Furthermore, by (2.8)

$$u(K_1^*;n,\alpha_2) \leqslant \varphi(\alpha_2,K_1^*+1)Q(n) < \varphi(\alpha_2,K_1^*+2)Q(n) < \varphi(\alpha_2,K_1^*+3)Q(n) < \cdots.$$

Therefore, by definition (2.1) of u,

$$u(K_1^*; n, \alpha_2) \leqslant u(K_1^* + 1; n, \alpha_2) < u(K_1^* + 2; n, \alpha_2) < u(K_1^* + 3; n, \alpha_2) < \cdots. \tag{2.32}$$

Since K_2^* is the smallest global solution to the problem $P(n, \alpha_2)$ defined by (2.1)–(2.4) with α there being replaced by α_2, we have

$$u(K_2^*; n, \alpha_2) \leqslant u(K_1^*; n, \alpha_2). \tag{2.33}$$

At last, by (2.32) and (2.33) and Lemma 2.1, (2.19) is obtained.

Now we are in a position to prove the conclusion that $K^*(n, \alpha)$ is nonincreasing with respect to $\alpha \in [2, \infty)$. Since $K^*(\cdot, \alpha)$ is right-continuous, we only need to show $K^*(n, \alpha)$ is nonincreasing with respect to $\alpha \in (2, \infty)$. This can be proved by contradiction. In fact, suppose that $K^*(n, \alpha)$ is not nonincreasing with respect to α, i.e. there exist $\bar{\alpha} > \underline{\alpha} > 2$ such that

$$K^*(n, \underline{\alpha}) < K^*(n, \bar{\alpha}). \tag{2.34}$$

Since $K^*(n, \alpha)$ is an integer function with respect to α, the above inequality implies

$$K^*(n, \underline{\alpha}) + 1 \leqslant K^*(n, \bar{\alpha}). \tag{2.35}$$

Define $I_0 = [\underline{\alpha}, \bar{\alpha}]$ and denote the left and right boundary points of I_0 as $\tilde{\alpha}_l(I_0)$ and $\tilde{\alpha}_r(I_0)$ respectively. According to (2.35), the interval I_0 has the property

$$K^*(n, \tilde{\alpha}_l(I_0)) + 1 \leqslant K^*(n, \tilde{\alpha}_r(I_0)). \tag{2.36}$$

Now we define an interval sequence $\{I_k\}$ $(k = 0, 1, \ldots)$ starting from I_0 by

$$I_{k+1} = \begin{cases} [\tilde{\alpha}_l(I_k), \frac{1}{2}(\tilde{\alpha}_l(I_k) + \tilde{\alpha}_r(I_k))] & \text{if } K^*(n, \tilde{\alpha}_l(I_k)) < K^*(n, \frac{1}{2}(\tilde{\alpha}_l(I_k) + \tilde{\alpha}_r(I_k))), \\ \frac{1}{2}(\tilde{\alpha}_l(I_k) + \tilde{\alpha}_r(I_k)), \tilde{\alpha}_r(I_k) & \text{otherwise}, \end{cases} \tag{2.37}$$

where $\tilde{\alpha}_l(I_k)$ and $\tilde{\alpha}_r(I_k)$ are the left and right boundary points of I_k, respectively. It is not difficult to prove, by induction, that the sequence $\{I_k\}$ has the following properties:

(a) $I_{k+1} \subseteq I_k$, $k = 0, 1, \ldots$.
(b) $\lim_{k\to\infty}(\tilde{\alpha}_r(I_k) - \tilde{\alpha}_l(I_k)) = \lim_{k\to\infty} 1/2^k(\bar{\alpha} - \underline{\alpha}) = 0$.
(c) $K^*(n, \tilde{\alpha}_l(I_k)) + 1 \leqslant K^*(n, \tilde{\alpha}_r(I_k))$, $k = 0, 1, \ldots$.

Therefore, there exists a unique $\tilde{\alpha} > 2$ satisfying

$$\tilde{\alpha}_l(I_k) \leqslant \tilde{\alpha} \leqslant \tilde{\alpha}_r(I_k), \quad k = 0, 1, \ldots \tag{2.38}$$

and

$$\lim_{k\to\infty} \tilde{\alpha}_r(I_k) = \lim_{k\to\infty} \tilde{\alpha}_l(I_k) = \tilde{\alpha}. \tag{2.39}$$

Since $K^*(n, \alpha)$ is an integer function and is right continuous with respect to α, there exists an integer $N > 0$ such that

$$K^*(n, \tilde{\alpha}_r(I_k)) = K^*(n, \tilde{\alpha}) \quad \text{for all } k > N. \tag{2.40}$$

By property (c) and (2.40), we have

$$K^*(n,\tilde{\alpha}_l(I_k))+1 \leqslant K^*(n,\tilde{\alpha}) \quad \text{for all } k > N$$

or

$$K^*(n,\tilde{\alpha}_l(I_k)) < K^*(n,\tilde{\alpha}) \quad \text{for all } k > N.$$

By (2.39), we know that the above inequality contradicts conclusion (2.19) with α_2 there being replaced by $\tilde{\alpha}$. So the lemma is proved. □

Lemma 2.4. *If $K^* = K^*(n,\alpha)$ is the smallest global solution to the problem $P(n,\alpha)$, then for any $\alpha \geqslant 2$, we have*

$$u(K^*;n,\bar{\alpha}) \leqslant u(K^*+1;n,\bar{\alpha}) < u(K^*+2;n,\bar{\alpha}) < \cdots \quad \textit{when } \bar{\alpha} \geqslant \alpha \tag{2.41}$$

and

$$u(0;n,\underline{\alpha}) > u(1;n,\underline{\alpha}) > \cdots > u(K^*;n,\underline{\alpha}) \quad \textit{when } 2 \leqslant \underline{\alpha} < \alpha. \tag{2.42}$$

Proof. Denote by $\bar{K}^*$ the smallest global solution to the problem $P(n,\bar{\alpha})$ defined by (2.1)–(2.4) with α there being replaced by $\bar{\alpha}$. By Lemma 2.1

$$u(\bar{K}^*;n,\bar{\alpha}) \leqslant u(\bar{K}^*+1;n,\bar{\alpha}) < u(\bar{K}^*+2;n,\bar{\alpha}) < \cdots. \tag{2.43}$$

On the other hand, for $\bar{\alpha} \geqslant \alpha$, by Lemma 2.3, we have

$$\bar{K}^* \leqslant K^*. \tag{2.44}$$

Combining (2.43) and (2.44) yields (2.41). The proof of (2.42) is similar and omitted. □

Lemma 2.5. *If a positive integer j and two scalars $\underline{\alpha}$ and $\bar{\alpha}$ $(2 \leqslant \underline{\alpha} < \bar{\alpha})$ satisfy*

$$u(j;n,\underline{\alpha}) > u(j+1;n,\underline{\alpha})$$

and

$$u(j;n,\bar{\alpha}) \leqslant u(j+1;n,\bar{\alpha}),$$

then there exists a scalar such that

$$b = \min\{\alpha \mid \alpha \geqslant 2; u(j;n,\alpha) \leqslant u(j+1;n,\alpha)\}. \tag{2.45}$$

Proof. We prove the conclusion by the following two steps.

First, we define a sequence of $[\beta_k,\gamma_k]$ $(k=0,1,\ldots)$ as follows: Set $\alpha_1 = (\underline{\alpha}+\bar{\alpha})/2$. If

$$u(j;n,\alpha_1) \leqslant u(j+1;n,\alpha_1),$$

then denote by $[\beta_0,\gamma_0]$ the interval $[\underline{\alpha},\alpha_1]$; otherwise denote by $[\beta_0,\gamma_0]$ the interval $[\alpha_1,\bar{\alpha}]$. Set $\alpha_2 = (\beta_0+\gamma_0)/2$. If

$$u(j;n,\alpha_2) \leqslant u(j+1;n,\alpha_2),$$

then denote by $[\beta_1, \gamma_1]$ the interval $[\beta_0, \alpha_2]$; otherwise denote by $[\beta_1, \gamma_1]$ the interval $[\alpha_2, \gamma_0]$. Repeating the above process, the sequence of $[\beta_k, \gamma_k]$ $(k = 0, 1, \ldots)$ is defined. Obviously, it has the following properties:

(1) $\beta_k \leqslant \beta_{k+1} < \gamma_{k+1} \leqslant \gamma_k$, $k = 0, 1, \ldots$.
(2) $\gamma_k - \beta_k = 1/2^{k+1}(\bar{\alpha} - \underline{\alpha})$.
(3) $u(j; n, \beta_k) > u(j+1; n, \beta_k)$ and $u(j; n, \gamma_k) \leqslant u(j+1; n, \gamma_k)$.
(4) $\lim_{k\to\infty} \gamma_k = \lim_{k\to\infty} \beta_k$.

Second, we define $b = \lim_{k\to\infty} \gamma_k$. From the above properties (1)–(4) and Lemma 2.2, we have

$$\beta_k \leqslant b \leqslant \gamma_k, \quad k = 0, 1, \ldots \tag{2.46}$$

and

$$u(j; n, b) \leqslant u(j+1; n, b). \tag{2.47}$$

So the conclusion is proved. □

3. The analytic expression

Next theorem gives an analytic expression of the solution to problem (2.1)–(2.4).

Theorem 3.1. *Consider the problem* $P(n, \alpha)$ (2.1)–(2.4) *with a fixed positive integer n. If* $\alpha \geqslant 2$, *then there exists the smallest global solution* $K^*(n, \alpha)$. *Furthermore, setting* $q = K^*(n, 2)$, *there are* $q + 1$ *scalars*

$$b_0 = b_0(n) \geqslant b_1 = b_1(n) \geqslant \cdots \geqslant b_q = b_q(n) = 2 \tag{3.1}$$

such that $K^*(n, \alpha)$, *as a function of* α, *can be expressed as*

$$K^*(n, \alpha) = \begin{cases} 0 & \text{when } \alpha \in [b_0(n), \infty), \\ 1 & \text{when } \alpha \in [b_1(n), b_0(n)), \\ \cdots & \\ q & \text{when } \alpha \in [b_q(n), b_{q-1}(n)), \end{cases} \tag{3.2}$$

where the interval $[b_j, b_{j-1})$ *is empty if* $b_j = b_{j-1}$, $j = 1, \ldots, q$.

Proof. The conclusion is proved by induction. As its first step, we show that there exists a scalar b_0 such that

$$K^*(n, \alpha) \begin{cases} = 0 & \text{when } \alpha \in [b_0, \infty), \\ > 0 & \text{when } \alpha \in [2, b_0). \end{cases} \tag{3.3}$$

First, let us prove the existence of b_0 defined by

$$b_0 = b_0(n) = \min\{\alpha \mid \alpha \geqslant 2; u(0; n, \alpha) \leqslant u(1; n, \alpha)\}. \tag{3.4}$$

Comparing $u(0; n, 2)$ with $u(1; n, 2)$, there are two cases: either

$$u(0; n, 2) \leqslant u(1; n, 2) \tag{3.5}$$

or

$$u(0;n,2) > u(1;n,2). \tag{3.6}$$

For the former case, $b_0 = 2$ obviously satisfies (3.4). As for the latter case, it is easy to find a sufficiently large $\tilde{\alpha}$ such that

$$u(0;n,\tilde{\alpha}) \leqslant u(1;n,\tilde{\alpha}). \tag{3.7}$$

According to (3.6) and (3.7), the existence of the scalar b_0 defined by (3.4) follows from Lemma 2.5.

Next we show that the scalar b_0 yields (3.3). From (3.4)

$$u(0;n,b_0) \leqslant u(1;n,b_0).$$

Hence, by Lemma 2.1, we get

$$K^*(n,b_0) = 0. \tag{3.8}$$

Furthermore, by (3.8) and Lemma 2.4, we conclude that when $\alpha \in [b_0, \infty)$

$$u(0;n,\alpha) \leqslant u(1;n,\alpha),$$

which implies that

$$K^*(n,\alpha) = 0. \tag{3.9}$$

On the other hand, by (3.4), we conclude that when $\alpha \in [2, b_0)$,

$$u(0;n,\alpha) > u(1;n,\alpha),$$

which implies that

$$K^*(n,\alpha) > 0. \tag{3.10}$$

Combining (3.9) and (3.10) yields the validity of (3.3). The first step of the induction is completed.

The second step begins with assuming that there exist $j+1$ scalars

$$b_i = \min\{\alpha \,|\, \alpha \geqslant 2; u(i;n,\alpha) \leqslant u(i+1;n,\alpha)\}, \quad i = 0,\ldots,j \tag{3.11}$$

such that

$$2 < b_j \leqslant b_{j-1} \leqslant \cdots \leqslant b_1 \leqslant b_0 \tag{3.12}$$

and

$$K^*(n,\alpha) \begin{cases} = 0 & \text{when } \alpha \in [b_0, \infty), \\ = 1 & \text{when } \alpha \in [b_1, b_0), \\ \cdots & \cdots \\ = j & \text{when } \alpha \in [b_j, b_{j-1}), \\ > j & \text{when } \alpha \in [2, b_j). \end{cases} \tag{3.13}$$

Let us show that there exists a scalar

$$b_{j+1} = \min\{\alpha \,|\, \alpha \geqslant 2; u(j+1;n,\alpha) \leqslant u(j+2;n,\alpha)\} \tag{3.14}$$

such that

$$2 \leqslant b_{j+1} \leqslant b_j \leqslant \cdots \leqslant b_1 \leqslant b_0 \tag{3.15}$$

and

$$K^*(n,\alpha)\begin{cases} =0 & \text{when } \alpha \in [b_0,\infty), \\ =1 & \text{when } \alpha \in [b_1,b_0), \\ \cdots & \cdots \\ =j & \text{when } \alpha \in [b_j,b_{j-1}), \\ =j+1 & \text{when } \alpha \in [b_{j+1},b_j), \\ >j+1 & \text{when } \alpha \in [2,b_{j+1}). \end{cases} \tag{3.16}$$

To show the existence of the scalar b_{j+1} defined by (3.14), consider the two cases

$$u(j+1;n,2) \leqslant u(j+2;n,2) \tag{3.17}$$

and

$$u(j+1;n,2) > u(j+2;n,2), \tag{3.18}$$

respectively. For case (3.17), b_{j+1} is obviously 2. For case (3.18), by (3.13), we have

$$K^*(n,b_j) = j. \tag{3.19}$$

Therefore, by Lemma 2.1,

$$u(j+1;n,b_j) < u(j+2;n,b_j). \tag{3.20}$$

According to (3.18) and (3.20), the existence of the scalar b_{j+1} defined by (3.14) follows from Lemma 2.5. In addition, by definition (3.14), we have

$$2 \leqslant b_{j+1} \leqslant b_j. \tag{3.21}$$

At last, we show by (3.16) or by (3.13) that when $b_{j+1} < b_j$

$$K^*(n,\alpha) = j+1 \quad \text{when } \alpha \in [b_{j+1},b_j) \tag{3.22}$$

and when $2 < b_{j+1}$

$$K^*(n,\alpha) > j+1 \quad \text{when } \alpha \in [2,b_{j+1}). \tag{3.23}$$

In fact, to show (3.23), on one hand, noticing (3.19), Lemma 2.4 and (3.11), when $\alpha < b_j$, we have

$$u(0;n,\alpha) > \cdots > u(j;n,\alpha) > u(j+1;n,\alpha). \tag{3.24}$$

Particularly, (3.24) with $\alpha = b_{j+1}$ yields that

$$u(0;n,b_{j+1}) > \cdots > u(j+1;n,b_{j+1}). \tag{3.25}$$

On the other hand, definition (3.14) implies that

$$u(j+1;n,b_{j+1}) \leqslant u(j+2;n,b_{j+1}). \tag{3.26}$$

By Lemma 2.1, combining (3.25) and (3.26) leads to

$$K^*(n,b_{j+1}) = j+1, \tag{3.27}$$

which implies, by Lemma 2.4, that when $\alpha \geqslant b_{j+1}$

$$u(j+1;n,\alpha) \leqslant u(j+2;n,\alpha). \tag{3.28}$$

Thus combining (3.24) and (3.28) yields that, when $\alpha \in [b_{j+1}, b_j)$

$$u(0,n,\alpha) > \cdots > u(j+1;n,\alpha) \leqslant u(j+2;n,\alpha). \tag{3.29}$$

Therefore, by Lemma 2.1, we conclude the validity of (3.22). To show (3.23), noticing that (3.27), Lemma 2.4 and (3.14) lead to when $\alpha < b_{j+1}$

$$u(0;n,\alpha) > \cdots > u(j+1;n,\alpha) > u(j+2;n,\alpha). \tag{3.30}$$

Hence, the validity of (3.23) follows.

Noting that in induction hypothesis (3.12), it is assumed that $2 < b_j$. However, in its conclusion (3.15), we get $2 \leqslant b_{j+1} \leqslant b_j$. So the sequence $b_0, b_1, \ldots$ is nonincreasing. Furthermore, we claim that its last element must be b_q, due to definition (3.14) with $j+1$ there being replaced by $q = K^*(n,2)$. □

For problem (2.1)–(2.4), Theorem 3.1 not only shows the existence of the analytic expression (3.2) of the solution, but also provides an approach by which the parameters q and $b_0, b_1, \ldots, b_q$ in (3.2) can be specified via finding a number of the smallest global solutions $K^*(n,\alpha)$ to (2.1)–(2.4) with different α. In fact, for a given dimension n, by Theorem 3.1, $q = K^*(n,2)$ and $b_q = 2$. In order to specify $b_0, \ldots, b_{q-1}$, suppose that the precision ε is given, which means that b_j^c $(j = 0, \ldots, q-1)$ are acceptable as approximates if

$$|b_j^c - b_j| \leqslant \varepsilon.$$

Thus b_0 is specified by the following steps:

Step 0: Set $b_l = 2$ and $b_r = 4$.
Step 1: Let $\bar{b} = (b_l + b_r)/2$ and obtain $K^*(n,\bar{b})$. If $K^*(n,\bar{b}) = 0$, then $b_r = \bar{b}$ and go to Step 3.
Step 2: Set $b_l = \bar{b}$. If $K^*(n,b_r) \geqslant 1$, then $b_r = 2b_r$.
Step 3: If $b_r - b_l \leqslant \varepsilon$, then $b_0 = \bar{b}$ and stop. Otherwise, go to Step 1.

As for specifying of b_i, $i = 1, 2, \ldots, q-1$, we only need to modify the above steps slightly as follows: In Step 0, $b_r = 4$ is replaced by $b_r = b_{i-1}$; In Step 1, $K^*(n,\bar{b}) = 0$ is replaced by $K^*(n,\bar{b}) = i$; In Step 2, "if $K^*(n,b_r) \geqslant 1$, then $b_r = 2b_r$" is deleted.

As an example, for $n = 200$ with the precision $\varepsilon = 0.01$, we get the expression

$$K^*(200,\alpha) = \begin{cases} 0 & \text{when } \alpha \in [4.66, \infty), \\ 1 & \text{when } \alpha \in [2.61, 4.66), \\ 2 & \text{when } \alpha \in [2, 2.61). \end{cases} \tag{3.31}$$

Note that Theorem 3.1 is useful to show the advantage of the corresponding Newton-PCG method where expression (3.2) is incorporated. For example, consider the case $n = 200$, $\alpha \in [\alpha_l, \alpha_h] = [2, 2.60]$ and compare the efficiency of Newton-PCG method with that of Newton's method by Ostrovskii's definition [6].

Definition 3.1. Efficiency Γ (Ostrovskii). Suppose that the sequence $\{x^0, x^1, \ldots, x^k, \ldots\}$ generated by an algorithm converges to the solution x^* with q-order ϱ, and the computation cost, required to compute x^{k+1} from x^k, is Q. Then the efficiency Γ of the algorithm is

$$\Gamma = \frac{\ln \varrho}{Q}. \tag{3.32}$$

Obviously, here the q-order of Newton's method is at most $\alpha_h = 2.60$. On the other hand, it can be shown that the average q-order of Newton-PCG method in $(1 + K^*)$ steps at least is $\alpha_l = 2$. Now let us turn to the computation cost. For simplicity, we neglect the cost to compute the Hessian and the gradient, and consider only the numbers of the multiplication operations involved in solving Newton equations. For Newton's method, the cost in every step is

$$Q_{\mathrm{N}}(n) = \frac{1}{6}n^3 + \frac{3}{2}n^2 - \frac{2}{3}n. \tag{3.33}$$

For Newton-PCG method , its average cost in $1 + K^*$ steps is

$$Q_{\text{N-PCG}}(n, K^*, \alpha) = \frac{Q_{\mathrm{N}}(n) + \sum_{m=1}^{K^*} \varphi(\alpha, m) Q_{\mathrm{SUB}}(n)}{1 + K^*}, \tag{3.34}$$

where $\varphi(\cdot, \cdot)$ is defined in (2.3), and $Q_{\mathrm{SUB}}(n) = 2n^2 + 6n + 2$ is the multiplicative operations in each PCG subiteration.

Denote Γ_{N} and $\Gamma_{\text{N-PCG}}$ as the efficiency of Newton's method and Newton-PCG method, respectively. Noticing $n = 200$, $\alpha \in [\alpha_l, \alpha_h] = [2, 2.60]$, and by (3.31), $K^* = 2$, it is easy to get the estimates

$$\Gamma_{\mathrm{N}} \leqslant \frac{\ln 2.60}{Q_{\mathrm{N}}(200)} \tag{3.35}$$

and

$$\Gamma_{\text{N-PCG}} \geqslant \frac{\ln 2}{Q_{\text{N-PCG}}(200, 2, 2.60)}. \tag{3.36}$$

So, by (3.33)–(3.36), we have

$$\Gamma_{\mathrm{N}} / \Gamma_{\text{N-PCG}} < 0.89,$$

which shows that Newton-PCG method is more efficient than Newton's method.

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