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The cluster problem revisited

Achim Wechsung · **Spencer D. Schaber** ·
Paul I. Barton

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Abstract In continuous branch-and-bound algorithms, a very large number of boxes near global minima may be visited prior to termination. This so-called cluster problem (Du and Kearfott, 1994) is revisited and a new analysis is presented. Previous results are confirmed, which state that at least second-order convergence of the relaxations is required to overcome the exponential dependence on the termination tolerance. Additionally, it is found that there exists a threshold on the convergence order pre-factor which can eliminate the cluster problem completely for second-order relaxations. This result indicates that, even among relaxations with second-order convergence, behavior in branch-and-bound algorithms may be fundamentally different depending on the pre-factor. A conservative estimate of the pre-factor is given for αBB relaxations.

Keywords Cluster problem · Global optimization · Convergence order · Convex relaxations

Mathematics Subject Classification (2000) 49M20 · 49M37 · 65K05 · 68Q25 · 90C26

1 Introduction

It is well known that branch-and-bound algorithms for continuous global optimization [5, 8] can visit a large number of small boxes in the vicinity of a global minimizer. This behavior was first discussed by Du and Kearfott [4] in the context of interval branch-and-bound methods and the authors coined the term *cluster problem* for this phenomenon. They provided

A. Wechsung
Process Systems Engineering Laboratory, Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave, Rm 66-363, Cambridge, MA 02139, USA.
E-mail: awechsun@mit.edu

S. D. Schaber
Process Systems Engineering Laboratory, Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave, Rm 66-363, Cambridge, MA 02139, USA.
E-mail: schaber@mit.edu

P. I. Barton
Process Systems Engineering Laboratory, Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave, Rm 66-464, Cambridge, MA 02139, USA.
Tel: +1 (617) 253-6526, Fax: +1 (617) 258-5042, E-mail: pib@mit.edu

an analysis to establish an upper bound on the number of boxes that cannot be fathomed by value dominance before the width of the boxes becomes smaller then a user specified tolerance. The authors were also the first to point out the importance of the convergence order of the bounding method (see Definition 1) in mitigating the cluster problem. Later, Neumaier [13] provided a similar analysis: it considers a hyperellipsoidal region around an unconstrained global minimizer, uses the determinant of the Hessian at the global minimizer instead of its smallest eigenvalue and introduces the proportionality constant for the volume of a hypersphere. Regardless, the result of the analysis is similar to Du and Kearfott [4] and stresses the importance of the convergence order. The main conclusion in these articles is that, in the worst case, at least second-order convergence is necessary to overcome the cluster problem. However, even with second-order convergence, the number of boxes still has exponential dependence on the problem dimension as Neumaier claims in [13]. Recently, Schöbel and Scholz [15] studied the worst-case behavior of branch-and-bound algorithms and gave an upper bound on the number of boxes needed for convergence that is very conservative.

If the minimizer coincides with the vertex of a box at some point in the branch-and-bound algorithm than an exponential number of boxes will contain this minimizer. The analysis presented below assumes, however, that boxes can be placed so that the minimizer is in the center of the box. Strategies such as back-boxing [17] or epsilon-inflation [10] can potentially avoid the former case. Also, see the discussion in [13, Ch. 15].

Here, the cluster problem is revisited and the analysis is refined. In particular, it is shown that the convergence order pre-factor is important: assuming second-order convergence, the exponential dependence on the problem dimension can be avoided if the pre-factor is sufficiently small and the minimizer is always in the interior of a box in the branch-and-bound tree. Thus, not all relaxations with second-order convergence are equal in higher dimensions. On the contrary, tightness of the relaxations, for which the pre-factor is a good measure, is very important. Also, it is demonstrated how to estimate the pre-factor conservatively for the αBB relaxations [1, 2, 9].

2 Analysis of the cluster problem

It is assumed that the reader is familiar with branch-and-bound algorithms for continuous global optimization [5, 8] and the construction and use of convex relaxations in such algorithms [1, 2, 11, 16].

Assumption 1 Suppose $D \subset \mathbb{R}^n$ is open, $C \subset D$ is convex and let $f : D \to \mathbb{R}$ be twice differentiable on D. Suppose that $\mathbf{x}^*$ is the *unique unconstrained* global minimum of f on C, so that $\nabla f(\mathbf{x}^*) = \mathbf{0}$ and suppose furthermore that $\nabla^2 f(\mathbf{x}^*)$ is positive definite.

Suppose $Z \subset \mathbb{R}^n$. The *set of all interval subsets* of Z is denoted by $\mathbb{I}Z$. The *width* of an n-dimensional interval X is defined as $w(X) = \max_{i=1,\ldots,n}(x_i^U - x_i^L)$.

Definition 1 Let a continuous convex relaxation of f on any $X \in \mathbb{I}C$ be given by $f_X^{cv} : X \to \mathbb{R}$. The relaxations are said to have *convergence order* $\beta \geq 1$ if there exists $K > 0$ such that

$$\min_{\mathbf{x}\in X} f(\mathbf{x}) - \min_{\mathbf{x}\in X} f_X^{cv}(\mathbf{x}) \leq K w(X)^{\beta}, \quad \forall X \in \mathbb{I}C. \tag{1}$$

Note that convergence order is typically defined as the difference of the width of the image of X under the enclosure of f and the width of the image of X under f [3, 12, 14]. However, Definition 1 is more natural for the purpose of this paper and the difference is unimportant for this argument.

Assumption 2 Let ε be the termination tolerance for the branch-and-bound algorithm and assume the algorithm has found the upper bound, $UBD_k = f(\mathbf{x}^*)$. Assume the algorithm terminates at iteration k when $UBD_k - LBD_k \leq \varepsilon$, where LBD_k is the current lower bound.

Lemma 1 *Let $X^* \in \mathbb{I}C$ be such that $\mathbf{x}^* \in X^*$. If the bound given by Definition 1 is sharp for all $X \in \mathbb{I}C$, then a necessary condition for termination of the branch-and-bound algorithm is*

$$w(X^*) \leq \left(\frac{\varepsilon}{K}\right)^{\frac{1}{\beta}}. \tag{2}$$

Proof At any iteration $LBD_k \leq \min_{\mathbf{x}\in X^*} f^{cv}_{X^*}(\mathbf{x}) \leq UBD_k$ holds. Thus, a necessary condition for termination is $UBD_k - \min_{\mathbf{x}\in X^*} f^{cv}_{X^*}(\mathbf{x}) \leq \varepsilon$. In the worst case, the bound on the underestimation by the relaxation in (1) is exact so that

$$UBD_k - \min_{\mathbf{x}\in X^*} f^{cv}_{X^*}(\mathbf{x}) = \min_{\mathbf{x}\in X^*} f(\mathbf{x}) - \min_{\mathbf{x}\in X^*} f^{cv}_{X^*}(\mathbf{x}) = Kw(X^*)^{\beta}.$$

Therefore, the algorithm terminates only if $Kw(X^*)^{\beta} \leq \varepsilon$. □

The following arguments adopt the convention that a node $\tilde{X}$ is fathomed by value dominance only when $\min_{\mathbf{x}\in\tilde{X}} f^{cv}_{\tilde{X}}(\mathbf{x}) > UBD_k$. In this situation, the stack is interpreted as representing the subset of C that can possibly contain global minima. This convention does not change the number of nodes processed by the branch-and-bound algorithm, it will only affect the number of nodes remaining on the stack at termination.

Lemma 2 *Define $\delta = \left(\frac{\varepsilon}{K}\right)^{\frac{1}{\beta}}$ and consider any node $\tilde{X} \in \mathbb{I}C$ with $w(\tilde{X}) \leq \delta$. Introduce the following partition of C:*

$$A = \{\mathbf{x} \in C : f(\mathbf{x}) - f(\mathbf{x}^*) > \varepsilon\},$$
$$B = \{\mathbf{x} \in C : f(\mathbf{x}) - f(\mathbf{x}^*) \leq \varepsilon\}.$$

Then, any node $\tilde{X} \subset A$ will be fathomed by value dominance.

Proof Suppose that $\tilde{X} \subset A$ so that $\min_{\mathbf{x}\in\tilde{X}} f(\mathbf{x}) - UBD_k = \min_{\mathbf{x}\in\tilde{X}} f(\mathbf{x}) - f(\mathbf{x}^*) > \varepsilon$. By construction of $\tilde{X}$, even in the worst case, Eq. (1) implies that

$$\min_{\mathbf{x}\in\tilde{X}} f(\mathbf{x}) - \min_{\mathbf{x}\in\tilde{X}} f^{cv}_{\tilde{X}}(\mathbf{x}) \leq K\delta^{\beta} = \varepsilon. \tag{3}$$

Since

$$\min_{\mathbf{x}\in\tilde{X}} f^{cv}_{\tilde{X}}(\mathbf{x}) \geq \min_{\mathbf{x}\in\tilde{X}} f_{\tilde{X}}(\mathbf{x}) - \varepsilon > UBD_k$$

it follows that $\tilde{X}$ will be fathomed by value dominance. □

Note that this result indicates that any node $\tilde{X} \subset A$ will be fathomed when or before $w(\tilde{X}) = \delta$. On the other hand, consider a node $\tilde{X}$ such that $\tilde{X} \cap B \neq \emptyset$ and $w(\tilde{X}) = \delta$ with δ as defined in Lemma 2. From $\tilde{X} \cap B \neq \emptyset$,

$$\min_{\mathbf{x}\in\tilde{X}} f(\mathbf{x}) - UBD_k = \min_{\mathbf{x}\in\tilde{X}} f(\mathbf{x}) - f(\mathbf{x}^*) \leq \varepsilon$$

so that in the worst case (3)

$$\min_{\mathbf{x}\in\tilde{X}} f^{cv}_{\tilde{X}}(\mathbf{x}) - UBD_k \leq 0.$$

In the worst case, such nodes will not be fathomed by value dominance.

Any node $\tilde{X}$ containing $\mathbf{x}^*$ will have $\tilde{X} \cap B \neq \emptyset$. In Lemma 1 it was argued that, when the convergence order bound is sharp, the node containing $\mathbf{x}^*$ must have width less than or equal to δ to guarantee termination. That is, in the worst case, B must be covered by nodes with $w(\tilde{X}) = \delta$ and none of them will be fathomed by value dominance.

2.1 Refinement of Neumaier's argument for a bound on the number of boxes necessary to cover B

Next, the number of boxes of width δ required to cover B is estimated. This argument will follow the idea presented by Neumaier [13]. Since f is twice differentiable at $\mathbf{x}^*$ and $\mathbf{x}^* \in \operatorname{int} C$, it follows that

$$f(\mathbf{x}) - f(\mathbf{x}^*) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^{\mathrm{T}}\nabla^2 f(\mathbf{x}^*)(\mathbf{x}-\mathbf{x}^*) + r(\mathbf{x}-\mathbf{x}^*),$$

so that B is given by

$$B = \left\{ \mathbf{x} \in C : \frac{1}{2}(\mathbf{x}-\mathbf{x}^*)^{\mathrm{T}}\nabla^2 f(\mathbf{x}^*)(\mathbf{x}-\mathbf{x}^*) + r(\mathbf{x}-\mathbf{x}^*) \leq \varepsilon \right\}. \tag{4}$$

(4) describes a nearly hyperellipsoidal region when $|r(\mathbf{x}-\mathbf{x}^*)| \ll \varepsilon$. This approximation becomes increasingly better for smaller ε because $|r(\mathbf{x}-\mathbf{x}^*)| \to 0$ as $\varepsilon \to 0$. Neumaier [13] compares the volume inside the hyperellipsoid, V, with the volume of a box to bound the number of boxes N that cover the interior of the hyperellipsoid from below. Denote $\Delta \equiv \det(\nabla^2 f(\mathbf{x}^*))$. Since

$$V(\varepsilon, n, \Delta) = \gamma_n \sqrt{\det\left[\left(\frac{\nabla^2 f(\mathbf{x}^*)}{2\varepsilon}\right)^{-1}\right]} = \gamma_n \sqrt{\frac{(2\varepsilon)^n}{\Delta}},$$

where $\gamma_n = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)}$ [7], it follows that

$$N \approx \frac{V(\varepsilon, n, \Delta)}{\delta^n} = \frac{\gamma_n \sqrt{\frac{(2\varepsilon)^n}{\Delta}}}{\left(\frac{\varepsilon}{K}\right)^{\frac{n}{\beta}}} = \gamma_n K^{\frac{n}{\beta}} \sqrt{\frac{2^n}{\Delta}} \varepsilon^{n\left(\frac{1}{2}-\frac{1}{\beta}\right)}. \tag{5}$$

This argument is valid only when boxes are able to approximate the volume inside the hyperellipsoid well. Moreover, as $n \to \infty$, $\gamma_n \to 0$ [6, 7]. For constant Δ and ε, it follows that $V \to 0$ as $n \to \infty$. Thus, this argument suggests that the cluster problem should disappear for sufficiently large n for any fixed K, β, and Δ.

Consider the volume inside a slightly smaller hyperellipsoid by replacing ε in (4) with $\varepsilon - \xi$ where $0 < \xi \ll \varepsilon$. It is easy to show that

$$\frac{V(\varepsilon, n, \Delta) - V(\varepsilon - \xi, n, \Delta)}{V(\varepsilon, n, \Delta)} = 1 - \sqrt{\left(1 - \frac{\xi}{\varepsilon}\right)^n} \to 1 \quad \text{as} \quad n \to \infty.$$

For higher dimensions, nearly all of the volume inside the hyperellipsoid is close to its surface and thus it is also distributed in space (i.e., *not* concentrated at the center). The estimate for N, which was obtained by comparing volumes as suggested by (5), may not lead to accurate results. A different analysis is necessary.

2.2 A new analysis of the cluster problem

A new argument for the number of boxes of width δ required to cover the volume inside the hyperellipsoid B will be given. In particular, two cases will be considered here. First, the simpler case of a hypersphere (i.e., $\nabla^2 f(\mathbf{x}^*) = \mathbf{I}$) will be treated. Second, the results are then generalized to the case of a hyperellipsoid.

Assumption 3 Assume that there exists only one box $\tilde{X}$ visited by the branch-and-bound algorithm such that $w(\tilde{X}) = \delta$ and $\mathbf{x}^* \in \tilde{X}$. Furthermore, assume that $\mathbf{x}^*$ is in the center of $\tilde{X}$.

Note that if $\mathbf{x}^*$ is in the interior of the box, but not in the center, then it will become necessary to use an apparent box width $\delta' \equiv 2\min_{i=1,\ldots,n}\{\tilde{x}_i^U - x_i^*, x_i^* - \tilde{x}_i^L\} \leq \delta$ in the following analysis instead.

For easier notation, a translated coordinate system $\mathbf{y} = \mathbf{x} - \mathbf{x}^*$ will be used hereafter, in which the considered approximation of B as the volume inside an hyperellipsoid is given by

$$\tilde{B} = \left\{\mathbf{y} : \frac{1}{2\varepsilon}\mathbf{y}^{\mathrm{T}}\nabla^2 f(\mathbf{0})\mathbf{y} \leq 1\right\}.$$

Denote a *box* centered at $\mathbf{y}_0$ with width ω by $\square_\omega(\mathbf{y}_0) \equiv \{\mathbf{y} : \|\mathbf{y} - \mathbf{y}_0\|_\infty \leq \frac{\omega}{2}\}$.

2.2.1 Case 1: Hypersphere

Lemma 3 *Suppose that* $\nabla^2 f(\mathbf{x}^*) = \mathbf{I}$ *and let* $r = \sqrt{2\varepsilon}$.

(a) *If* $\delta \geq 2r$, *then let* $N = 1$.
(b) *If* $\frac{2r}{\sqrt{m-1}} > \delta \geq \frac{2r}{\sqrt{m}}$ *where* $m \in \mathbb{N}$, $m \leq n$, $2 \leq m \leq 18$, *then let*

$$N = \sum_{i=0}^{m-1} 2^i \binom{n}{i} + 2n\left\lceil \frac{m-9}{9} \right\rceil.$$

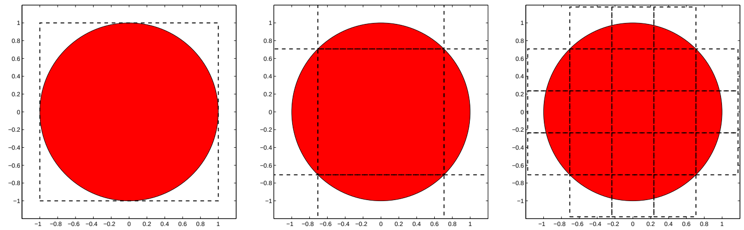
(c) *Otherwise let*

$$N = \left\lceil \frac{2r}{\delta\sqrt{2}} \right\rceil^{n-1} \left(\left\lceil \frac{2r}{\delta\sqrt{2}} \right\rceil + 2n \left\lceil \frac{r - \frac{r}{\sqrt{2}}}{\delta} \right\rceil \right).$$

Then, N *is an upper bound on the number of boxes with width* δ *required to cover* $\tilde{B}$.

Proof By definition, $\tilde{B} = \left\{\mathbf{y} : \frac{1}{2\varepsilon}\mathbf{y}^{\mathrm{T}}\mathbf{I}\mathbf{y} = \frac{1}{2\varepsilon}\mathbf{y}^{\mathrm{T}}\mathbf{y} \leq 1\right\}$ describes the region inside a hypersphere about the origin with radius $r = \sqrt{2\varepsilon}$.

(a) Suppose that $\delta \geq 2r$. One finds immediately that $N = 1$ since $\mathbf{y} \in \tilde{B}$ implies $\mathbf{y} \in \square_\delta(\mathbf{0})$ as $\|\mathbf{y}\|_\infty \leq \|\mathbf{y}\|_2$ and $\delta \geq 2r$.
(b) Suppose that $1 < m \leq 18$ and $\delta \geq \frac{2r}{\sqrt{m}}$. Place a box with width δ at the center of the hypersphere. Let $\mathbf{e}_i$ be any n-vector whose components are 0 except i of the entries which are $\pm\frac{\delta}{2}$. Such an $\mathbf{e}_i$ represents the $(n-i)$-faces of the hypercube. In particular, each $\mathbf{e}_i$ is the midpoint of such a face and it is well known that an n-dimensional hypercube has $F(n,i) \equiv 2^i\binom{n}{i}$ of these. Hence, $\mathbf{e}_i$ is representative of $F(n,i)$ directions.
It will be argued that, in addition to the central box, placing a single box along each of the $\mathbf{e}_1, \ldots, \mathbf{e}_m$ directions is sufficient to cover $\tilde{B}$.



(a) (b) (c)

Fig. 1: Illustration of different cases for a circle where dashed regions show boxes required to cover $\tilde{B}$

If $\delta > \frac{2r}{\sqrt{m}}$ then $\frac{2r}{\delta\sqrt{m}}\mathbf{e}_m \notin \tilde{B}$. If $\delta = \frac{2r}{\sqrt{m}}$, then $\frac{2r}{\delta\sqrt{m}}\mathbf{e}_m \in \Box_\delta(\mathbf{0})$ and also $\frac{2r}{\delta\sqrt{m}}\mathbf{e}_m \in \partial\tilde{B}$. As a consequence, faces lower than the $(n-m)$-face need not be considered as they do not intersect the hypersphere whereas additional boxes must be placed in the direction of all faces from the $(n-m+1)$-face up to the $(n-1)$-face to cover $\tilde{B}$.

Set $\delta = \frac{2r}{\sqrt{m}}$, the width of the smallest permissible box. Next, consider the shortest distance from $\frac{2r}{\delta\sqrt{i}}\mathbf{e}_i$, which is a point on the surface of the hypersphere, to the surface of the central box in the ∞-norm: $\frac{r}{\sqrt{i}} - \frac{\delta}{2} = \frac{r}{\sqrt{i}} - \frac{r}{\sqrt{m}}$. When this distance is smaller than δ, then one box suffices to cover the remaining parts of the hypersphere in the $\mathbf{e}_i$ direction. This holds true for any $i = 2, \ldots, m$ and $m \leq 18$. When $m > 9$, then two boxes must be placed in each of the $\mathbf{e}_1$ directions, however.

(c) Otherwise, the central region inside the hypersphere cannot be covered by a single box. Instead, a number of boxes that grows exponentially with n is necessary to fill the central region. Additional boxes must be placed along the coordinate axes so that $N = m^n + 2nm^{n-1}\left\lceil \frac{1}{\delta}\left(r - \frac{r}{\sqrt{2}}\right)\right\rceil$ where m is the smallest integer so that $m\delta \geq \frac{2r}{\sqrt{2}}$. Thus, the result follows. $\square$

Note that the number of boxes presented for the second case in Lemma 3 is $O(n^{m-1})$. Also, while it is possible to construct tighter bounds on N for the case $m > 18$, it becomes much more involved. In particular, it becomes necessary to place more than one box in the $\mathbf{e}_i$, $i > 1$ direction, which complicates the geometry. Roughly speaking, these boxes will only touch each other in a lower dimensional face leaving parts of $\tilde{B}$ uncovered, hence, requiring additional boxes.

The different cases are illustrated for $n = 2$ and $m = 2$ in Figure 1.

2.2.2 Case 2: Hyperellipsoid

The results in Lemma 3 will now be generalized to a hyperellipsoid by dropping the assumption that $\nabla^2 f(\mathbf{x}^*) = \mathbf{I}$.

Theorem 1 *Let $\lambda_1 > 0$ be the smallest eigenvalue of $\nabla^2 f(\mathbf{x}^*)$ and $r = \sqrt{\frac{2\varepsilon}{\lambda_1}}$.*

(a) If $\delta \geq 2r$ or, equivalently, if

$$\left(\frac{\varepsilon}{K}\right)^{\frac{1}{\beta}} \geq 2\sqrt{\frac{2\varepsilon}{\lambda_1}},$$

then let $N = 1$.

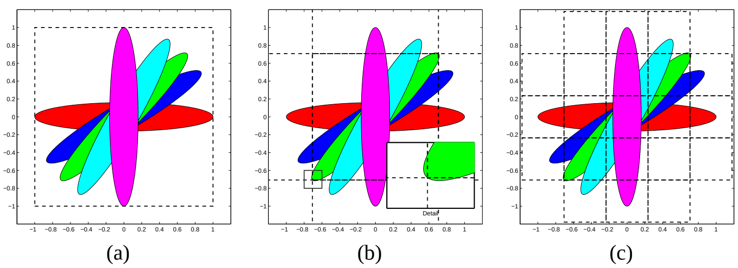


Fig. 2: Illustration of different cases for an ellipse where dashed regions show boxes required to cover $\tilde{B}$

(b) Suppose that $\frac{2r}{\sqrt{m-1}} > \delta \geq \frac{2r}{\sqrt{m}}$ *where* $m \in \mathbb{N}$, $m \leq n$, $2 \leq m \leq 18$ *or, equivalently,*

$$\frac{2\sqrt{2\varepsilon}}{\sqrt{(m-1)\lambda_1}} > \left(\frac{\varepsilon}{K}\right)^{\frac{1}{\beta}} \geq \frac{2\sqrt{2\varepsilon}}{\sqrt{m\lambda_1}}.$$

Then let

$$N = \sum_{i=0}^{m-1} 2^i \binom{n}{i} + 2n \left\lceil \frac{m-9}{9} \right\rceil.$$

(c) Otherwise, let

$$N = \left\lceil 2K^{\frac{1}{\beta}} \varepsilon^{\left(\frac{1}{2}-\frac{1}{\beta}\right)} \lambda_1^{-\frac{1}{2}} \right\rceil^{n-1} \left(\left\lceil 2K^{\frac{1}{\beta}} \varepsilon^{\left(\frac{1}{2}-\frac{1}{\beta}\right)} \lambda_1^{-\frac{1}{2}} \right\rceil + 2n \left\lceil (\sqrt{2}-1) K^{\frac{1}{\beta}} \varepsilon^{\left(\frac{1}{2}-\frac{1}{\beta}\right)} \lambda_1^{-\frac{1}{2}} \right\rceil \right).$$

Then, N is an upper bound on the number of boxes with width δ required to cover $\tilde{B}$.

Proof Suppose $\mathbf{y} \in \tilde{B}$ so that $\mathbf{y}^{\mathrm{T}} \nabla^2 f(\mathbf{0}) \mathbf{y} \leq 2\varepsilon$. By Rayleigh's principle,

$$0 \leq \lambda_1 \mathbf{y}^{\mathrm{T}} \mathbf{y} \leq \mathbf{y}^{\mathrm{T}} \nabla^2 f(\mathbf{0}) \mathbf{y} \leq 2\varepsilon$$

so that $\lambda_1 \mathbf{y}^{\mathrm{T}} \mathbf{y} \leq 2\varepsilon$. Thus, $\tilde{B} \subset \left\{ \mathbf{z} : \frac{\lambda_1}{2\varepsilon} \mathbf{z}^T \mathbf{z} \leq 1 \right\}$, the volume inside a hypersphere with radius $r = \sqrt{2\varepsilon\lambda_1^{-1}}$. Hence, Lemma 3 with $r = \sqrt{2\varepsilon\lambda_1^{-1}}$ can be applied and it provides an upper bound for N. $\square$

The different cases are illustrated for $n = 2$ and $m = 2$ in Figure 2.

3 Discussion of Theorem 1

Studying the expressions derived above for N, two characteristics are noteworthy:

- the variation of N with ε depends on the value of β and
- the influence of K on the behavior of N.

Both will be discussed in more detail. First, consider the functional dependence of N on ε for different β.

Case	N
$K \le \frac{\lambda_1}{8}$	1
$\frac{\lambda_1}{8} < K \le \frac{\lambda_1}{4}$	$1+2n$
$\frac{\lambda_1}{4} < K \le \frac{3\lambda_1}{8}$	$1+2n^2$
$\frac{3\lambda_1}{8} < K \le \frac{\lambda_1}{2}$	$1+\frac{8}{3}n-3n^2+\frac{4}{3}n^3$
$\vdots$	$\vdots$
$K > \frac{9\lambda_1}{4}$	$\left\lceil 2\sqrt{K\lambda_1^{-1}}\right\rceil^{n-1}\left(\left\lceil 2\sqrt{K\lambda_1^{-1}}\right\rceil + 2n\left\lceil (\sqrt{2}-1)\sqrt{K\lambda_1^{-1}}\right\rceil\right)$

Table 1: Summary of results for number of boxes required to cover $\tilde{B}$ when $\beta = 2$

1. When $\beta = 1$ and K not necessarily small, then $N \propto \left(\frac{1}{\varepsilon}\right)^{\frac{n}{2}}$. The number of boxes required to cover the hyperellipsoid will grow rapidly as the convergence tolerance ε is decreased—the well-known cluster problem.
2. When $\beta = 2$, then N is independent of ε for any value of K, i.e., the number of boxes required to cover the hyperellipsoid is insensitive to ε.
3. When $\beta = 3$ and K not necessarily small, then $N \propto \varepsilon^{\frac{n}{6}}$, and the number of boxes required to cover the hyperellipsoid will decrease with decreasing ε. Note that this does not necessarily mean that the total number of nodes required for termination decreases with the tolerance, because this analysis only estimates the number of nodes to cover B, which itself decreases in size as ε is decreased.

These observations agree with the results found in the literature [4, 13].

Second, assume that $\beta = 2$ and focus on how K parametrizes the behavior of N. Table 1 summarizes these results for the case $\beta = 2$. When K is sufficiently small, i.e., $K \le \frac{\lambda_1}{8}$, the cluster problem is completely absent ($N = 1$). Recall that λ_1 denotes the smallest eigenvalue of $\nabla^2 f(\mathbf{x}^*)$. When λ_1 is small, this bound may only hold for $K \ll 1$. Depending on the magnitude of K, N is polynomial (of varying degree) in n. For example, when $K \le \frac{\lambda_1}{4}$, then N grows linearly with problem size and when $K \le \frac{3\lambda_1}{8}$ the number of boxes grows quadratically with n. Both cases are remarkable as they suggest a fundamentally different behavior of different relaxations with second-order convergence each depending on these thresholds for K. Prior analyses of the cluster problem [4, 13] stop short of explicitly drawing this conclusion.

4 Estimating the convergence order pre-factor K

In light of the discussion above, it is interesting not only to determine the convergence order of different relaxations but also to estimate the pre-factor K. Here, αBB relaxations [1, 2, 9] will be considered as a simple illustration.

In the most general case, αBB relaxations of f on $X \in \mathbb{I}C$ are defined as

$$f_X^{\mathrm{cv}}(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{n} \alpha_i(X)(x_i^L - x_i)(x_i^U - x_i)$$

where $\alpha_i(X)$ are non-negative reals that are sufficiently large to guarantee convexity of f_X^{cv} on X. Different methods have been proposed to calculate α_i [1, 9] and $\alpha_i(X)$ can be updated as X changes. Regardless of the method, an upper bound on K can be obtained by the following result.

Theorem 2 *Consider αBB relaxations of f and suppose C is an interval. Let $\alpha \equiv \max_{i=1,\ldots,n} \alpha_i$ where α_i has been calculated on C. Then, $\beta = 2$ and $K \leq \frac{1}{4}\alpha n$.*

Proof It is easy to see that, for any $X \in \mathbb{I}C$,

$$\begin{aligned}
\min_{\mathbf{x}\in X} f(\mathbf{x}) - \min_{\mathbf{x}\in X} f_X^{cv}(\mathbf{x}) &= \min_{\mathbf{x}\in X} f(\mathbf{x}) - \min_{\mathbf{x}\in X} \left(f(\mathbf{x}) + \sum_{i=1}^{n} \alpha_i (x_i^L - x_i)(x_i^U - x_i) \right) \\
&\leq \min_{\mathbf{x}\in X} f(\mathbf{x}) - \min_{\mathbf{x}\in X} f(\mathbf{x}) - \min_{\mathbf{x}\in X} \sum_{i=1}^{n} \alpha_i (x_i^L - x_i)(x_i^U - x_i) \\
&= \sum_{i=1}^{n} \alpha_i \left(\frac{w(X_i)}{2} \right)^2 \leq \frac{1}{4}\alpha n (w(X))^2.
\end{aligned}$$

Thus, it follows that $\beta = 2$ and that $K = \frac{1}{4}\alpha n$ is a conservative estimate of the pre-factor. □

In Section 3 it was remarked that $K \leq \frac{9\lambda_1}{4}$ must hold for a second-order relaxation in order to prevent the exponential growth of N with n. For αBB relaxations this condition translates to $\alpha \leq \frac{9\lambda_1}{n}$. Recall that $\lambda_1 > 0$ is the smallest eigenvalue of $\nabla^2 f(\mathbf{x}^*)$, not the smallest eigenvalue of $\nabla^2 f$ on C. Note also that Theorem 2 does not indicate whether αBB relaxations can achieve this criterion. Furthermore, the result assumes that α_i does not change with X.

Suppose now that we construct a new α on each interval visited. A note-worthy feature of αBB relaxations is that $\alpha(X^1) \geq \alpha(X^2)$ for intervals X^1, X^2 such that $X^1 \supset X^2$. Hence, when α is re-computed for each X^l in a sequence of nested intervals, the corresponding sequence $\{\alpha^l\}$, and thus also the sequence of pre-factors $\{K^l\}$, is monotonically decreasing. This explains the behavior reported in [3, Figures 1, 2] for αBB relaxations with variable α. It is not possible, however, to argue that in general $\lim_{l\to\infty} \alpha^l = 0$, which would imply a super-quadratic order of convergence, see [3, Figure 3] for a counter-example.

Lastly, note that αBB relaxations coincide with f on X when $\alpha(X) = 0$ so that the lower bound is exact in this case.

5 Conclusion

The analysis of the cluster problem has been revisited in this paper. Prior results that reveal the dependence of the cluster problem on the convergence order β and the termination tolerance ε have been verified. Furthermore, even for relaxations with $\beta = 2$, the new analysis indicates fundamentally different scaling behavior depending on the value of K, the pre-factor in the convergence order. Thus, tighter relaxations can lead to dramatic improvements in mitigating the cluster problem.

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