Convergence under Subdivision and Complexity of Polynomial Minimization in the Simplicial Bernstein Basis*

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Abstract

In this article, we address the question of minimizing a real polynomial over the standard simplex. This problem can be solved with a branch-and-bound method, using the Bernstein form of the polynomial. Such methods have been widely studied from a numerical point of view, and refinements have been proposed to speed up the computational time. We are here interested in the basic branch-and-bound algorithm (and its complexity), which has the advantage to lead to certified proofs.

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1 Introduction

In this article we study the problem of approximating the minimum value of a polynomial on the standard simplex, which can be stated as follows:

$$\begin{aligned} &\min f(x) \\ \text{s.t.} \quad & x \in \Delta \end{aligned} \tag{$\mathcal{P}$}$$

where f is a polynomial of degree d in k variables. Here, Δ stands for the standard simplex, defined as:

$$\Delta = \{x \in \boldsymbol{R}^k \mid x \geqslant 0 \text{ and } \sum_{i=1}^{k} x_i \leqslant 1\}.$$

Problem ($\mathcal{P}$) (and its complexity) is widely studied (see [4, 5] and the references therein), and has several applications in financial engineering (portfolio optimization),

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life sciences (genetics, population dynamics) and graph theory. For example, as pointed out in [5], the *maximum stable set problem* is a particular case of Problem $(\mathcal{P})$. Consequently, Problem $(\mathcal{P})$ is an NP-hard problem, already for polynomials of degree 2.

Numerical methods can generally be of real interest to tackle NP-hard problems of polynomial optimization (see [9, 7, 14] in the general framework of polynomial optimization, and [4, 5] in the context of polynomial optimization over a simplex). However, stability problems can occur with such methods, and it can be difficult to control the numerical precision, which can lead to an incertitude concerning the obtained results. This is especially the case when one seeks a *formal proof*, *i.e.* a proof in which every logical inference has been checked (see [6] for an example of a formal proof involving optimization problems).

We study here the complexity of a basic branch-and-bound method. This algorithm makes use of the *simplicial Bernstein basis* and its *range enclosing property*, which has proved to be useful in bounding ranges of polynomials over domains (see, for example, [8], [13]).

2 Background

We now give the necessary background on the simplicial Bernstein basis (see the textbook [16] for further details).

2.1 Simplicial Bernstein Basis

We first recall the definition of a simplex:

Definition 2.1. *Let $\mathbf{v}_0, \ldots, \mathbf{v}_k$ be $k+1$ points of $\boldsymbol{R}^k$ ($k \geq 1$).*

The ordered list $V = [\mathbf{v}_0, \ldots, \mathbf{v}_k]$ is called simplex of vertices $\mathbf{v}_0, \ldots, \mathbf{v}_k$.

The realization $|V|$ of the simplex V is the set of $\boldsymbol{R}^k$ defined as the convex hull of the points $\mathbf{v}_0, \ldots, \mathbf{v}_k$.

If the points $\mathbf{v}_0, \ldots, \mathbf{v}_k$ are affinely independent, the simplex V is said to be non-degenerate.

Notation 2.2. *Throughout the article $V = [\mathbf{v}_0, \ldots, \mathbf{v}_k]$ will denote a non-degenerate simplex of $\boldsymbol{R}^k$, or, by abuse of notation, its realization $|V|$.*

Let $\lambda_0, \ldots, \lambda_k$ be the associated barycentric coordinates to V, *i.e.* the linear polynomials of $\boldsymbol{R}[\mathbf{X}] = \boldsymbol{R}[X_1, \ldots, X_k]$ such that

$$\sum_{i=0}^{k} \lambda_i(\mathbf{X}) = 1 \qquad \text{and} \qquad \forall \mathbf{x} \in \boldsymbol{R}^k,\ \mathbf{x} = \lambda_0(\mathbf{x})\mathbf{v}_0 + \cdots + \lambda_k(\mathbf{x})\mathbf{v}_k.$$

Recall that V is characterized by its barycentric coordinates as follows:

$$V = \bigcap_{i=0}^{k} \{\mathbf{x} \in \boldsymbol{R}^k | \lambda_i(\mathbf{x}) \geq 0\}.$$

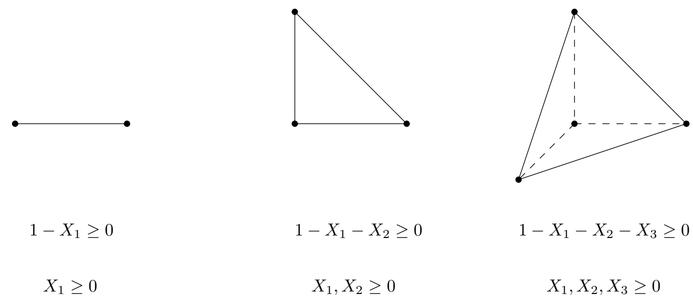

Figure 1: Standard simplices and associated barycentric coordinates in dimension $1, 2, 3$.

Example 2.3. *Let* $(\mathbf{e}_1, \ldots, \mathbf{e}_k)$ *denote the canonical basis of* $\boldsymbol{R}^k$*, and* $\mathbf{0} = (0, \ldots, 0)$ *the origin. The simplex* $\Delta = [\mathbf{0}, \mathbf{e}_1, \ldots, \mathbf{e}_k]$ *is called standard simplex of* $\boldsymbol{R}^k$*.*

The following notation will be useful afterwards:

Notation 2.4. *For every multi-index* $\alpha = (\alpha_0, \ldots, \alpha_k) \in \boldsymbol{N}^{k+1}$*, we write* $|\alpha| = \alpha_0 + \cdots + \alpha_k$*.*

The Bernstein polynomials are defined as follows:

Definition 2.5. *Let* d *be a natural number. The Bernstein polynomials of degree* d *with respect to* V *are the polynomials* $\left(B_\alpha^d\right)_{|\alpha|=d}$*, where:*

$$B_\alpha^d = \binom{d}{\alpha} \lambda^\alpha = \frac{d!}{\alpha_0! \ldots \alpha_k!} \prod_{i=0}^{k} \lambda_i^{\alpha_i} \in \boldsymbol{R}[\mathbf{X}].$$

The Bernstein polynomials of degree d w.r.t. V form a basis of the vector-space of the polynomials of degree $\leq d$. Thus, every polynomial f of degree $\leq d$ can be uniquely written as

$$f = \sum_{|\alpha|=d} b_\alpha(f, d, V) B_\alpha^d,$$

and the numbers $b_\alpha(f, d, V)$ are called Bernstein coefficients of f of degree d with respect to V. We denote by $b(f, d, V)$ the list of all the Bernstein coefficients $b_\alpha(f, d, V)$ (in any order).

2.2 Control Net

The Bernstein coefficients of a polynomial f give some geometric information, which can be expressed in terms of the so-called control points:

Definition 2.6. *Let* $V = [\mathbf{v}_0, \ldots, \mathbf{v}_k]$ *be a non-degenerate simplex of* $\boldsymbol{R}^k$*,* $f \in \boldsymbol{R}[\mathbf{X}]$ *a polynomial of degree* $\leq d$ *and* $b_\alpha(f, d, V)$ $(|\alpha| = d)$ *its Bernstein coefficients of degree* d *w.r.t.* V*.*

- *The grid points of degree* d *associated to* V *are the points*

$$\mathbf{v}_\alpha(d, V) = \frac{\alpha_0 \mathbf{v}_0 + \cdots + \alpha_k \mathbf{v}_k}{d} \in \boldsymbol{R}^k \quad (|\alpha| = d).$$

- *The control points associated to f of degree d w.r.t. V are the points*

$$\mathbf{C}_\alpha = \big(\mathbf{v}_\alpha(d,V), b_\alpha(f,d,V)\big) \in \boldsymbol{R}^{k+1} \quad (|\alpha| = d).$$

The control points of f form its control net of degree d.

- *The discrete graph of f of degree d w.r.t. V is formed by the points* $\Big(\mathbf{v}_\alpha(d,V), f\big(\mathbf{v}_\alpha(d,V)\big)\Big)_{|\alpha|=d}$.

We then have the following classical properties (see [16] for proofs):

Proposition 2.7. *Keeping the same notations, we have:*

(i) **linear precision:** *if* $\deg f \leq 1$*, then:*

$$\forall |\alpha| = d,\ b_\alpha(f,d,V) = f(\mathbf{v}_\alpha(d,V)).$$

(ii) **interpolation at the vertices:** *if* $(\mathbf{e}_0,\ldots,\mathbf{e}_k)$ *denotes the canonical basis of* $\boldsymbol{R}^{k+1}$*, then:*

$$\forall i \in \{0,\ldots,k\},\ b_{d\mathbf{e}_i}(f,d,V) = f(\mathbf{v}_i).$$

(iii) **convex hull property:** *the graph of f is contained in the convex hull of its associated control points.*

(iv) **range enclosure property:** *Consequently,*

$$\forall x \in V,\ \min_{|\alpha|=d} b_\alpha(f,d,V) \leq f(x) \leq \max_{|\alpha|=d} b_\alpha(f,d,V).$$

We then aim at comparing the discrete graph of f to its control net.

In order to compare the control net to the discrete graph of a polynomial, we will make use of the so-called *second differences*:

Definition 2.8. *Let* $(\mathbf{e}_0,\ldots,\mathbf{e}_k)$ *be the standard basis of* $\boldsymbol{R}^{k+1}$ *(with the convention* $\mathbf{e}_{-1} = \mathbf{e}_k$*), and* $V = [\mathbf{v}_0,\ldots,\mathbf{v}_k]$ *a simplex of* $\boldsymbol{R}^k$*.*
For $|\gamma| = d-2$ *and* $0 \leq i < j \leq k$*, define the quantity (where b_α stands for $b_\alpha(f,d,V)$):*

$$\nabla^2 b_{\gamma,i,j}(f,d,V) = b_{\gamma+\mathbf{e}_i+\mathbf{e}_{j-1}} + b_{\gamma+\mathbf{e}_{i-1}+\mathbf{e}_j} - b_{\gamma+\mathbf{e}_{i-1}+\mathbf{e}_{j-1}} - b_{\gamma+\mathbf{e}_i+\mathbf{e}_j}.$$

The collection $\nabla^2 b(f,d,V) = \big(\nabla^2 b_{\gamma,i,j}(f,d,V)\big)_{\substack{|\gamma|=d-2\\ 0\leq i<j\leq k}}$ *forms the second differences of f of degree d w.r.t. V.*

Notation 2.9. *Let* $\left\|\nabla^2 b(f,d,V)\right\|_\infty$ *denote the quantity* $\max\limits_{\substack{|\gamma|=d-2\\ 0\leq i<j\leq k}} |\nabla^2 b_{\gamma,i,j}(f,d,V)|$.

In [10], the author obtains an explicit bound on the gap between the control net and the discrete graph of a polynomial, namely:

Theorem 2.10. *With the previous notations, we have:*

$$\max_{|\alpha|=d} \left| f\big(\mathbf{v}_\alpha(d,V)\big) - b_\alpha(f,d,V)\right| \leq \frac{\left\lfloor \dfrac{d^2 k(k+2)}{12} \right\rfloor}{2d} \left\|\nabla^2 b(f,d,V)\right\|_\infty.$$

Remark 2.11. *This result generalizes results from [11] (dimension 1) and [17] (dimension 2).*

2.3 Convergence under Subdivision

In the following, we study the behavior of the Bernstein coefficients of a polynomial when subdividing a simplex.

Let $f \in \boldsymbol{R}[\mathbf{X}]$ be a polynomial of degree d over the standard simplex V. Assume that V has been subdivided, *i.e.*

$$V = V^1 \cup \cdots \cup V^s,$$

where the interiors of the simplices V^i $(1 \leq i \leq s)$ are disjoint.

The expansion of f in the Bernstein basis of degree d associated with each subsimplex V^i can be computed using only convex combinations of its Bernstein coefficients w.r.t V. This can be done by successive calls to the De Casteljau algorithm ([15],[16]), which we recall for the readers' convenience.

Notation 2.12. *If $V = [\mathbf{v}_0, \ldots, \mathbf{v}_k]$ is a simplex of $\boldsymbol{R}^k$ and $M \in \boldsymbol{R}^k$, the simplices $V^{[i]}$ $(i = 0, \ldots, k)$ are defined as follows:*

$$V^{[i]} = [\mathbf{v}_0, \ldots, \mathbf{v}_{i-1}, M, \mathbf{v}_{i+1}, \ldots, \mathbf{v}_k].$$

In what follows, if $\alpha \in \boldsymbol{N}^{k+1}$ and $0 \leq i \leq k$, we write

$$\widehat{\alpha_i} = (\alpha_0, \ldots, \alpha_{i-1}, 0, \alpha_{i+1}, \ldots, \alpha_k).$$

Recall that the barycentric coordinates of M w.r.t. V are denoted by

$$(\lambda_0(M), \ldots, \lambda_k(M)).$$

The standard basis of $\boldsymbol{R}^{k+1}$ is denoted by $(\mathbf{e}_0, \ldots, \mathbf{e}_k)$.

Algorithm 2.13 (De Casteljau)**.**

INPUT: *a simplex V, the Bernstein expansion $b(f, d, V)$ of a polynomial f of degree d over V, and a point $M \in \boldsymbol{R}^k$.*

OUTPUT: *the Bernstein expansions $b(f, d, V^{[i]})$ of f associated to the subsimplices $V^{[i]}$, for every $i \in \{0, \ldots, k\}$.*

ALGORITHM:
$\forall |\alpha| = d,\ b^{(0)}_\alpha \leftarrow b_\alpha(f, d, V).$

for $\ell = 1, \ldots, d$ ***do***
  for $|\alpha| = d - \ell$ ***do***
    $b^{(\ell)}_\alpha \leftarrow \sum_{p=0}^{k} \lambda_p(M) b^{(\ell-1)}_{\alpha+\mathbf{e}_p}$
  end for
end for

return $b_\alpha(f, d, V^{[i]}) = b^{(\alpha_i)}_{\widehat{\alpha_i}}$ $(|\alpha| = d,\ i = 0, \ldots, k)$.

If $U = [\mathbf{u}_0, \ldots, \mathbf{u}_k]$ is a subsimplex of V, then the Bernstein expansion $b(f, d, U)$ can be computed from $b(f, d, V)$ by $k + 1$ successive calls to De Casteljau's algorithm at the points $\mathbf{u}_0, \ldots, \mathbf{u}_k$. In each call, only convex combinations of the Bernstein coefficients $b(f,d,V)$ are involved. This process is called *reparametrization*.

In the following, we will focus on subdivision schemes that reduce the diameter in the following sense:

Definition 2.14. *Let V be a non-degenerate simplex of $\boldsymbol{R}^k$, S be a subdivision scheme (i.e. a rule for subdividing any simplex), and $S(V) = V^1 \cup \cdots \cup V^s$ be the resulting subdivision of V.*

- *The mesh of V, denoted by $m(V)$, is its diameter.*

  The mesh of $S(V)$, denoted by $m(S(V))$, is the largest mesh among the subsimplices V^i.
- *S is said to have a shrinking factor $0 < C < 1$ if for every simplex V,*

$$m(S(V)) \leq C \times m(V).$$

- *$S^N(V)$ denotes the subdivision of V obtained after N successive subdivision steps.*

Example 2.15. *The so-called* binary splitting *consists in splitting each simplex at the midpoint of its (not necessary unique) longest edge. In this case, a call to De Calsteljau algorithm can be executed faster than for an arbitrary point in the interior of the simplex ([14]), and generates the Bernstein expansion of f over the two subsimplices. Since a non-degenerate simplex has $\frac{k(k+1)}{2}$ edges, the following is easy to see:*

Lemma 2.16. *After at most $\dfrac{k(k+1)}{2}$ steps of binary splitting of a simplex of diameter h, the diameter of the subsimplices is less than $h/2$.*

In other words, the subdivision scheme consisting in $\dfrac{k(k+1)}{2}$ steps of binary splitting has a shrinking factor $\frac{1}{2}$.

When subdividing a simplex (so that the diameters of the subsimplices converge to 0), the control net of a polynomial converges to its discrete graph: this well-known property is called *convergence under subdivision*. In [10], the author deduces from Theorem 2.10 an *explicit* bound implying convergence under subdivision:

Theorem 2.17. *Let W be a subsimplex of a simplex V.*

Then, for all $|\alpha| = d$, we have:

$$\left| f\left(\mathbf{v}_\alpha(d,W)\right) - b_\alpha(f,d,W) \right| \leq m(W)^2 d \frac{k^2(k+1)(k+2)^2(k+3)}{576} \left\| \nabla^2 b(f,d,V) \right\|_\infty .$$

Remark 2.18. *Note that the previous theorem implies that the rate of convergence is quadratic in the diameter of the subsimplices, as already shown in [3]. The improvement here is that the bound is explicit in terms of the dimension, the degree and the Bernstein expansion of f over V.*

3 Polynomial Minimization over the Standard Simplex

When minimizing a polynomial f over a non-degenerate simplex V, one can use an approach based on the simplicial Bernstein basis. Indeed, the range enclosure property leads to a lower bound of f on V. By repeatedly subdividing V, the minimum of f over V can then be approximated within any desired accuracy. This procedure is called *Bernstein branch and bound* method. It can be used not only to numerically minimize a polynomial over a simplex, but also to obtain certified formal proofs. Polynomial minimization is a NP-hard problem, so the complexity of such a procedure is high. In this section, we bound the number of needed subdivision steps.

Remark 3.1. *In [12, 13], the problem of minimizing a polynomial in Bernstein form is also studied. However, the authors use the so-called tensorial Bernstein basis (see [16] for details), in which polynomials can be expanded with respect to boxes* $[a_1, b_1] \times \cdots \times [a_k, b_k] \subset \boldsymbol{R}^k$. *One advantage of using the simplicial Bernstein basis is to deal with a simpler representation of polynomials.*

3.1 Branch and Bound Algorithm

Let V be a non-degenerate simplex and S be a subdivision scheme. In the process of minimizing a polynomial, the subdivision scheme as described above continues even for subsimplices where the minimum cannot occur. In order to delete such subsimplices, so that unnecessary subdivisions are avoided, one can use the simple *cut-off test*:

Lemma 3.2 (cut-off test)**.** *Let W be a subsimplex of V, and $f^\star$ an upper bound on the minimum of f over V.*

If $\min_{|\alpha|=d} b_\alpha\big(f, d, W\big) > f^\star$, then the minimum of f cannot occur in W. Hence, W can be deleted from the list of simplices to be subdivided.

Remark 3.3. *From a certified point of view, computing the minimum means computing a lower and an upper bound of it; computing the minimizers means giving a list of subsimplices that contain all the minimizers.*

Note also that in the output of the following algorithm, a simplex V is always given together with the Bernstein expansion $b_V = b(f, d, V)$, the minimum Bernstein coefficient

$$m_V = \min_{|\alpha|=d} b_\alpha(f, d, V)$$

and, when relevant, the value f_V defined as

$$f_V = \min\big(f\big(\mathbf{v}_\alpha(d, V)\big), b_{d\mathbf{e}_0}(f, d, V), \ldots, b_{d\mathbf{e}_k}(f, d, V)\big)\,,$$

where α satisfies $b_\alpha(f, d, V) = m_V$.

From Properties (ii) (interpolation at the vertices) and (iv) (range enclosure) of Proposition 2.7, one can obviously deduce that

$$m_V \leq \min_{x \in V} f(x) \leq f_V. \tag{3.1}$$

We now present a *certified version* of the usual Bernstein branch and bound algorithm.

Algorithm 3.4 (Branch and bound algorithm).

INPUT:

- *the list* $b_\Delta = (b_\alpha(f, d, \Delta))_{|\alpha|=d}$ *of the Bernstein coefficients of a polynomial* $f \in \boldsymbol{R}[\mathbf{X}]$ *of degree* d *with respect to the standard simplex* Δ *of* $\boldsymbol{R}^k$
- *a subdivision scheme* S *with shrinking factor* $C < 1$
- *a precision* $\varepsilon > 0$

OUTPUT:

- *A lower bound* $m^\star$ *and an upper bound* $f^\star$ *of the minimum* m *of* f *over* Δ*, such that* $f^\star - m^\star \leq \varepsilon$
- *A collection of subsimplices of* Δ *that contain all the possible minimizers.*
- *A collection of rejected subsimplices, that are sure not to contain any minimizer.*

ALGORITHM:

$f^\star \leftarrow f_\Delta$
$L \leftarrow \{(\Delta, b_\Delta, m_\Delta, f^\star)\}$
$S \leftarrow \emptyset$
$R \leftarrow \emptyset$

while $L \neq \emptyset$ ***do***
  Pick the first item (V, b_V, m_V, f_V) *of* L*, and delete it from* L*.*
  $f^\star \leftarrow \min(f^\star, f_V)$
  if $m_V > f^\star$ ***then***
    Add (V, b_V, m_V) *to* R*.* {*cut-out test*}
  else
    if $f_V - m_V \leq \varepsilon$ ***then***
      Add (V, b_V, m_V, f_V) *to* S*.*
    else
      Subdivide V*.*
      for W *in* $S(V)$ ***do***
        Compute the Bernstein expansion of f *over* W*.*
        Add the items (W, b_W, m_W, f_W) *to* L*.*
        $f^\star \leftarrow \min(f^\star, f_W)$
      end for
    end if
  end if
end while

Discard from S *and place into* R *all the subsimplices* V *such that* $m_V > f^\star$*.*

$m^\star \leftarrow \min_{V \in S} m_V$

return $m^\star$ {*lower bound on the minimum of* f *over* Δ}

return $f^\star$ {*upper bound on the minimum of* f *over* Δ}

return S {*subsimplices that contain all the minimizers*}

return R {*subsimplices that are sure to contain no minimizer*}

Remark 3.5.

- *Algorithm 3.4 is certified in the following sense: from the Bernstein expansions of f over the subsimplices in S and R, one can read the proof that:*
  - *(i) The minimum of f over Δ satisfies:*

    $$m^\star \leq \min_{x\in\Delta} f(x) \leq f^\star.$$

  - *(ii) The minimizers belong to subsimplices from the list S.*
  - *(iii) No subsimplex from R contains a minimizer.*

  This can lead to a formal proof, and be checked by proof assistants (e.g. Coq, [1]), or implemented in a theorem prover like PVS ([2]).
- *$f\big(\mathbf{v}_\alpha(d,V)\big)$ can be evaluated by means of the De Casteljau's algorithm ([15],[16]). When doing this, it generates a subdivision of V that can be used to speed up the subdivision process (note that the subdivision scheme S still has to have a shrinking factor $C < 1$)*
- *If ε is to be lowered, one can use the result of a former instance of this algorithm to meet the new accuracy requirement.*
- *If $m^\star = f_V$ for a simplex $V \in S$, then the* exact *minimum of f over Δ has been computed by Algorithm 3.4, and an exact minimizer is easily computed.*

Proof of Algorithm 3.4. The proof is an immediate consequence of Lemma 3.2 and Equation (3.1). The number of subdivision steps is finite, and is bounded in the next section. □

3.2 Number of Subdivision Steps

We now prove that Algorithm 3.4 stops, and bound the number of subdivision steps:

Theorem 3.6. *Let $f \in \boldsymbol{R}[\mathbf{X}]$ be a polynomial of degree d, and S a subdivision scheme with shrinking factor $C < 1$.*

Let $\varepsilon > 0$ a real number, and N an integer satisfying:

$$\frac{1}{C^{2N}} \geq d\frac{k^2(k+1)(k+2)^2(k+3)}{288\,\varepsilon}\left\|\nabla^2 b(f,d,\Delta)\right\|_\infty.$$

Then Algorithm 3.4 needs at most N subdivision steps.

Proof. It is sufficient to show that $|f_V - m_V| \leq \varepsilon$ for each subsimplex $V \in S^N(\Delta)$.

Let $V \in S^N(V)$ be such a simplex, and α a multi-index such that $m_V = b_\alpha(f,d,V)$. Then:

$$\begin{aligned}
|f_V - m_V| &= f_V - m_V \\
&\leq f\big(\mathbf{v}_\alpha(d,V)\big) - b_\alpha(f,d,V) \\
&\leq m(V)^2 d\frac{k^2(k+1)(k+2)^2(k+3)}{576}\left\|\nabla^2 b(f,d,\Delta)\right\|_\infty \quad \text{(Th. 2.17)} \\
&\leq \big(C^N S(\Delta)\big)^2 d\frac{k^2(k+1)(k+2)^2(k+3)}{576}\left\|\nabla^2 b(f,d,\Delta)\right\|_\infty \\
&\leq C^{2N} d\frac{k^2(k+1)(k+2)^2(k+3)}{288}\left\|\nabla^2 b(f,d,\Delta)\right\|_\infty,
\end{aligned}$$

where the last inequality comes from the fact that $S(\Delta) = \sqrt{2}$. This allows us to conclude. □

Remark 3.7. *The bound in Theorem 3.6 does not take into account the cut-off test, which in practice drastically improves the computational time.*

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