Optimality of a gradient bound for polyhedral Wachspress coordinates

Michael S. Floater

Department of Mathematics, University of Oslo,
PO Box 1053, Blindern, 0316 Oslo, Norway
email: michaelf@math.uio.no

Abstract. In a recent paper with Gillette and Sukumar an upper bound was derived for the gradients of Wachspress barycentric coordinates in simple convex polyhedra. This bound provides a shape-regularity condition that guarantees the convergence of the associated polyhedral finite element method for second order elliptic problems. In this paper we prove the optimality of the bound using a family of hexahedra that deform a cube into a tetrahedron.

Keywords: Barycentric coordinates, Wachspress coordinates, polyhedral finite element method

1 Introduction

There is growing interest in using generalized barycentric coordinates for finite element methods on polygonal and polyhedral meshes [3, 7, 8, 13, 9, 1]. In order to establish the convergence of such methods one needs to derive an upper bound on the gradients of the coordinate functions in each polygonal or polyhedral cell. Such an upper bound was derived recently in [1] for Wachspress' rational coordinates in simple convex polytopes in $\mathbb{R}^d$. By 'simple' here we mean a polytope in which every vertex has exactly d incident faces. Thus in the important cases $\mathbb{R}^2$ and $\mathbb{R}^3$, this means any convex polygon in $\mathbb{R}^2$, but in $\mathbb{R}^3$, it means a convex polyhedron in which every vertex has three incident faces. For example, among the Platonic solids, the tetrahedron, cube, and dodecahedron are simple polyhedra, while the octahedron and icosahedron are not.

In the 2-D polygonal case, the upper bound of [1] was shown there to be optimal. The purpose of this note is to prove that the bound is also optimal in 3-D. The proof uses a one-parameter family of hexahedra (which are simple) in which the three faces incident on one vertex approach coplanarity. The family continuously deforms a cube, until, in the limiting case, it becomes a tetrahedron.

It is hoped that this work might motivate further research on this topic. For example, finding a similar, simple gradient bound for Wachspress coordinates in non-simple polyhedra is an open question, as is a corresponding bound for other types of coordinates such as mean value coordinates.

2 Barycentric coordinates on polyhedra

Let $P \subset \mathbb{R}^3$ be a convex polyhedron, viewed as an open set, with V and F its vertices and faces; see Figure 1. We call a set of functions $\phi_{\mathbf{v}} : P \to \mathbb{R}$, $\mathbf{v} \in V$,

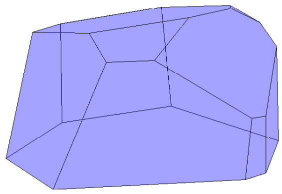

Fig. 1. A simple convex polyhedron

barycentric coordinates if they are non-negative, and if, for any $\mathbf{x} \in P$,

$$\sum_{\mathbf{v}\in V} \phi_{\mathbf{v}}(\mathbf{x})\mathbf{v} = \mathbf{x}, \qquad \sum_{\mathbf{v}\in V} \phi_{\mathbf{v}}(\mathbf{x}) = 1. \tag{1}$$

It has been shown [2] that such functions extend continuously to the boundary ∂P of P. They have the Lagrange property at the vertices, i.e., $\phi_{\mathbf{v}}(\mathbf{u}) = \delta_{\mathbf{vu}}$, $\mathbf{v}, \mathbf{u} \in V$, and they are linear along each edge of P. The function $\phi_{\mathbf{v}}$ is zero on any face f that does not have $\mathbf{v}$ as a vertex. If $f \in F$ is a face and $\mathbf{x}$ is any point in f,

$$\sum_{\mathbf{v}\in V_f} \phi_{\mathbf{v}}(\mathbf{x})\mathbf{v} = \mathbf{x}, \qquad \sum_{\mathbf{v}\in V_f} \phi_{\mathbf{v}}(\mathbf{x}) = 1, \tag{2}$$

where $V_f \subset V$ is the set of vertices of f.

Suppose next that $\phi_{\mathbf{v}} \in C^1(P)$ for all $\mathbf{v} \in V$, which is, for example, the case for Wachspress coordinates [10, 6, 11, 12, 5] and mean value coordinates [2, 4], both of which are in $C^\infty(P)$. Then we could consider using the $\phi_{\mathbf{v}}$ as shape functions over a domain partitioned into convex polyhedra, as in [3, 7, 1]. In order to establish a convergence theory for such a method we need to consider the vertex-based interpolation operator I of a function $u : \overline{P} \to \mathbb{R}$ given by

$$I(u) := \sum_{\mathbf{v}\in V} u(\mathbf{v})\phi_{\mathbf{v}}. \tag{3}$$

With $|\cdot|$ the Euclidean norm in $\mathbb{R}^3$, we need to derive an upper bound on

$$|\nabla I(u)(\mathbf{x})|, \qquad \mathbf{x} \in P,$$

in terms of u and the geometry of P. Observe that for $\mathbf{x} \in P$,

$$|\nabla I(u)(\mathbf{x})| \le \sum_{\mathbf{v}\in V} |u(\mathbf{v})\nabla\phi_{\mathbf{v}}(\mathbf{x})| \le \lambda(\mathbf{x}) \max_{\mathbf{v}\in V} |u(\mathbf{v})|, \tag{4}$$

where

$$\lambda(\mathbf{x}) := \sum_{\mathbf{v}\in V} |\nabla\phi_{\mathbf{v}}(\mathbf{x})|, \tag{5}$$

and so

$$\sup_{\mathbf{x}\in P} |\nabla I(u)(\mathbf{x})| \leq \Lambda \max_{\mathbf{v}\in V} |u(\mathbf{v})|,$$

where

$$\Lambda := \sup_{\mathbf{x}\in P} \lambda(\mathbf{x}).$$

Thus the function $\lambda : P \to \mathbb{R}$ plays a role similar to that of the Lebesgue function in the theory of polynomial interpolation, and Λ acts like the Lebesgue constant. The goal is to derive an upper bound on Λ in terms of the geometry of P.

3 Wachspress coordinates for polyhedra

Wachspress' rational coordinates for convex polygons and polyhedra were developed and studied by Wachspress, Warren and others [10, 6, 11, 12, 5]. In [11], Warren generalized the 2-D coordinates of Wachspress to simple convex polyhedra. The derivation was based on the so-called 'adjoint' of the polyhedron. In [12], Warren et al. derived the same coordinates in a different way, avoiding the adjoint, as follows. For each face $f \in F$, let $\mathbf{n}_f \in \mathbb{R}^3$ denote its unit outward normal, and for any $\mathbf{x} \in P$, let $h_f(\mathbf{x})$ denote the perpendicular distance of $\mathbf{x}$ to f, which can be expressed as the scalar product

$$h_f(\mathbf{x}) = (\mathbf{v} - \mathbf{x}) \cdot \mathbf{n}_f,$$

for any vertex $\mathbf{v} \in V$ belonging to f. For each vertex $\mathbf{v} \in V$, let f_1, f_2, f_3 be the three faces incident to $\mathbf{v}$, and for $\mathbf{x} \in P$, let

$$w_{\mathbf{v}}(\mathbf{x}) = \frac{\det(\mathbf{n}_{f_1}, \mathbf{n}_{f_2}, \mathbf{n}_{f_3})}{h_{f_1}(\mathbf{x}) h_{f_2}(\mathbf{x}) h_{f_3}(\mathbf{x})}, \tag{6}$$

where it is understood that f_1, f_2, f_3 are ordered such that the determinant in the numerator is positive. Here, for vectors $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathbb{R}^3$,

$$\det(\mathbf{a}, \mathbf{b}, \mathbf{c}) := \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}.$$

Thus the ordering of f_1, f_2, f_3 must be anticlockwise around $\mathbf{v}$, seen from outside P. In this way, $w_{\mathbf{v}}(\mathbf{x}) > 0$, and it was shown in [12] that the functions

$$\phi_{\mathbf{v}}(\mathbf{x}) := \frac{w_{\mathbf{v}}(\mathbf{x})}{\sum_{\mathbf{u}\in V} w_{\mathbf{u}}(\mathbf{x})} \tag{7}$$

are barycentric coordinates, i.e., satisfy (1). Some matlab code for evaluating these coordinates and their gradients can be found in [1].

4 Gradient bound

The following bound on Λ was derived in [1] for Wachspress coordinates $\phi_{\mathbf{v}}$ for a simple polyhedron P: if

$$h_* := \min_{f \in F} \min_{\mathbf{v} \in V \setminus V_f} h_f(\mathbf{v}), \tag{8}$$

the minimal perpendicular distance between vertices and faces of P, then

$$\Lambda \leq \frac{6}{h_*}. \tag{9}$$

The significance of this is that it implies convergence for the polyhedral finite element method applied to second order elliptic problems with shape-regularity parameter $\kappa := \mathrm{diam}(P)/h_*$.

We will establish the optimality of (9) by constructing a family of hexahedra $\{P_\epsilon\}$ containing a vertex $\mathbf{v}$ such that

$$\lim_{\epsilon \to 0} h_* \lambda(\mathbf{v}) = 6. \tag{10}$$

In fact we do this for λ defined with respect to *any* barycentric coordinates that are C^1 at the vertices of P. Though the particular constant 6 in (10) is not essential, (10) clearly shows the dependency of Λ on h_*.

We recall first a preliminary result of [1]. Let $\mathbf{v}$ be some vertex of P, and let $\mathbf{w}_1$, $\mathbf{w}_2$, $\mathbf{w}_3$ be its three neighbours, and define the three vectors $\mathbf{e}_k = \mathbf{w}_k - \mathbf{v}$, k=1,2,3. It was shown in [1] that for any barycentric coordinates $\phi_{\mathbf{u}}$, $\mathbf{u} \in V$, that are C^1 at $\mathbf{v}$,

$$\lambda(\mathbf{v}) = |\nabla \phi_{\mathbf{v}}(\mathbf{v})| + \sum_{i=1}^{3} |\nabla \phi_{\mathbf{w}_i}(\mathbf{v})|, \tag{11}$$

with

$$\nabla \phi_{\mathbf{w}_1}(\mathbf{v}) = \frac{1}{D}\mathbf{e}_2 \times \mathbf{e}_3, \quad \nabla \phi_{\mathbf{w}_2}(\mathbf{v}) = \frac{1}{D}\mathbf{e}_3 \times \mathbf{e}_1, \quad \nabla \phi_{\mathbf{w}_3}(\mathbf{v}) = \frac{1}{D}\mathbf{e}_1 \times \mathbf{e}_2,$$

$$\nabla \phi_{\mathbf{v}}(\mathbf{v}) = -\frac{1}{D}(\mathbf{e}_2 \times \mathbf{e}_3 + \mathbf{e}_3 \times \mathbf{e}_1 + \mathbf{e}_1 \times \mathbf{e}_2), \quad \text{and} \quad D = \det(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3).$$

This is a consequence of the linearity of the coordinates on the edges of P, their Lagrange property at the vertices, and the assumption of C^1 regularity at $\mathbf{v}$.

From these formulas we obtain

Lemma 1. *Suppose the vertex* $\mathbf{v}$ *is such that*

$$|\mathbf{e}_1| = |\mathbf{e}_2| = |\mathbf{e}_3|, \qquad \mathbf{e}_2 \cdot \mathbf{e}_3 = \mathbf{e}_3 \cdot \mathbf{e}_1 = \mathbf{e}_1 \cdot \mathbf{e}_2,$$

and $h_* = h_f(\mathbf{w}_3)$*, where* f *is the face containing* $\mathbf{v}$*,* $\mathbf{w}_1$*, and* $\mathbf{w}_2$*. Then,*

$$h_* \lambda(\mathbf{v}) = 3 + R,$$

where $R = (|\mathbf{e}_2 \times \mathbf{e}_3 + \mathbf{e}_3 \times \mathbf{e}_1 + \mathbf{e}_1 \times \mathbf{e}_2|)/|\mathbf{e}_1 \times \mathbf{e}_2|$.

This follows from the formula (11) and the fact that $h_f(\mathbf{w}_3) = -\mathbf{e}_3 \cdot \mathbf{n}_f$ and $\mathbf{n}_f = -(\mathbf{e}_1 \times \mathbf{e}_2)/|\mathbf{e}_1 \times \mathbf{e}_2|$. Thus, to prove the optimality of the bound (9) it is sufficient to find a sequence of simple polyhedra with a vertex $\mathbf{v}$ satisfying the conditions of the lemma and such that $R \to 3$.

5 A family of hexahedra

We achieve the convergence $R \to 3$ with the following family of hexahedra. In analogy with the unit cube, we will use the typical notation $\mathbf{v}_{ijk}$, $0 \le i, j, k \le 1$, for the eight vertices of the hexahedron, with the connectivity it implies. For any ϵ with $0 < \epsilon < 3\sqrt{2}$, let P_ϵ be the hexahedron with vertices, in increasing z coordinate,

$$\begin{aligned}
&\mathbf{v}_{000} = (0,0,0),\\
&\mathbf{v}_{100} = (2,0,\epsilon), \quad \mathbf{v}_{010} = (-1,\sqrt{3},\epsilon), \quad \mathbf{v}_{001} = (-1,-\sqrt{3},\epsilon),\\
&\mathbf{v}_{110} = r(1,\sqrt{3},2\epsilon), \quad \mathbf{v}_{011} = r(-2,0,2\epsilon), \quad \mathbf{v}_{101} = r(1,-\sqrt{3},2\epsilon),\\
&\mathbf{v}_{111} = (0,0,3\sqrt{2}),
\end{aligned}$$

where $r = 2\sqrt{2}/(\sqrt{2}+\epsilon)$. One can check that the six 'faces' really are faces, i.e., planar, by verifying that the two determinants

$$\begin{aligned}
&\det(\mathbf{v}_{100} - \mathbf{v}_{000}, \mathbf{v}_{110} - \mathbf{v}_{000}, \mathbf{v}_{010} - \mathbf{v}_{000}),\\
&\det(\mathbf{v}_{101} - \mathbf{v}_{001}, \mathbf{v}_{100} - \mathbf{v}_{001}, \mathbf{v}_{110} - \mathbf{v}_{001}),
\end{aligned}$$

are zero. One can also verify that if $\epsilon = \sqrt{2}$ then $r = 1$ and $P_{\sqrt{2}}$ is a cube with side length $\sqrt{6}$. Figure 2 shows P_ϵ for four values of ϵ, decreasing from $\sqrt{2}$.

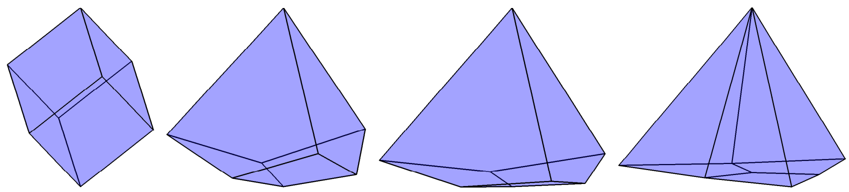

Fig. 2. Hexahedron P_ϵ, $\epsilon = \sqrt{2}(1, 0.25, 0.1, 0.01)$

Considering again the ratio R of the lemma, let

$$\mathbf{v} = \mathbf{v}_{000}, \quad \mathbf{w}_1 = \mathbf{v}_{100}, \quad \mathbf{w}_2 = \mathbf{v}_{010}, \quad \mathbf{w}_3 = \mathbf{v}_{001},$$

in which case the conditions of the lemma hold for small ϵ. We compute

$$\mathbf{e}_1 \times \mathbf{e}_2 = (2,0,\epsilon) \times (-1,\sqrt{3},\epsilon) = (-\sqrt{3}\epsilon, -3\epsilon, 2\sqrt{3}),$$

$$\mathbf{e}_2 \times \mathbf{e}_3 = (2\sqrt{3}\epsilon, 0, 2\sqrt{3}), \qquad \mathbf{e}_3 \times \mathbf{e}_1 = (-\sqrt{3}\epsilon, 3\epsilon, 2\sqrt{3}),$$

and so

$$\mathbf{e}_1 \times \mathbf{e}_2 + \mathbf{e}_2 \times \mathbf{e}_3 + \mathbf{e}_3 \times \mathbf{e}_1 = (0,0,6\sqrt{3}).$$

Therefore,

$$R = \frac{6\sqrt{3}}{2\sqrt{3(1+\epsilon^2)}} = \frac{3}{\sqrt{1+\epsilon^2}} \to 3 \qquad \text{as } \epsilon \to 0.$$

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