Voronoi diagrams, Delaunay triangulations and their optimality criteria in multidimensional numerical integration

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Outline

What exactly are triangulations?

- Simplex is the convex hull of any $d+1$ affinely independent points in $\mathbb{R}^d$.
- Circumsphere of a simplex is the sphere which passes through all the vertices of the simplex.
- A polytope is the convex hull of a finite set of points in $\mathbb{R}^d$.

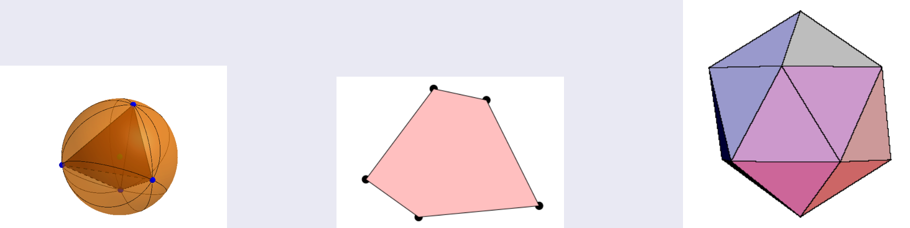


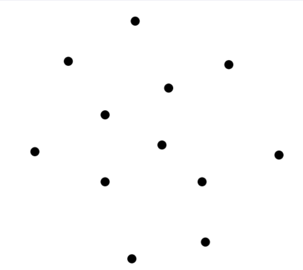
Figure: Left: Circumsphere of a Tetrahedron. Middle: The convex hull of 5 points in the plane. Right: 3D polytope

What exactly are triangulations?

A triangulation of a given set of points $X \subset \mathbb{R}^d$ is a partition into simplices such that

- **Union Property**: the union of all these simplices equals conv(X).
- **Intersection Property**: any two simplices do not intersect or intersect along a common face.

Example of a set of 12 points and one of its triangulation



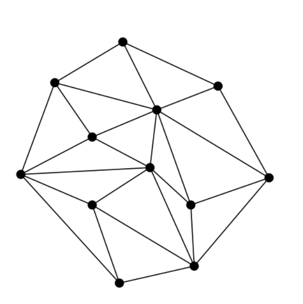


Figure: Titre commun

The following example is not a triangulation

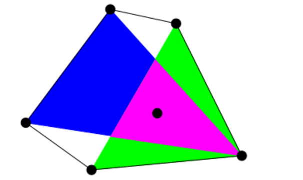


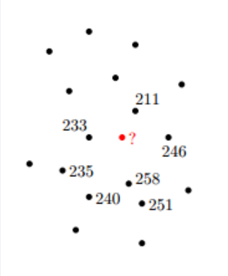
Figure: The intersection property is not satisfied.

Motivation: Terrains by interpolation

To build a model of the terrain surface, we can start with a number of sample points where we know the height.

Motivation: Terrains by interpolation

How do we interpolate the height at other points?



Triangulation today is used for many purposes, including navigation,

- Nearest neighbor interpolation.
- Piecewise linear interpolation by a triangulation.
- Moving windows interpolation.
- Natural neighbor interpolation

Motivation: Why triangulations?

Triangulations are widely used as a standard tool to decompose complicated objects into simple objects. Triangulations have applications in a large number of fields. Some examples are the following:

- Numerics: Finite Elements Method, F.V.M., ...
- Computer Graphics: Raytracing.
- Algebraic Geometry: Connection to Toric Varieties
- Algebra: Polynomial System Solving.
- Homotopy Theory: Structure of Loop Spaces.
- . . . .

Existence of Triangulations

Theorem

Every finite set of points in $\mathbb{R}^d$ admits at least one Triangulation.

What about uniqueness?

Let us have a set of points in $\mathbb{R}^d$. We can create many triangulations on them.

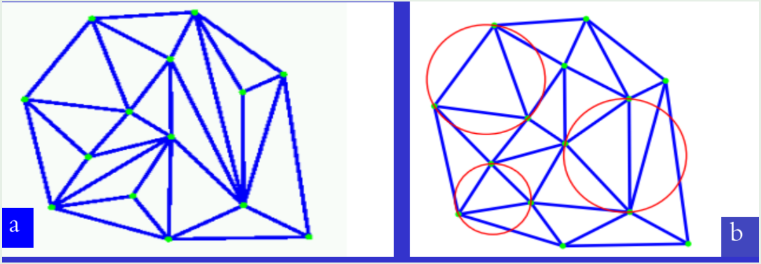


Figure: Example : Two triangulations of the same set of 14 points.

- (a) is any triangulation.
- (b) satisfies the empty interior sphere condition.

What about the number of triangulations ?

There are of course many possible different triangulations of a given set of points

Theorem

The number of triangulations of a convex polygon with $n+2$ sides into n triangles is the Catalan number C_n, where

$$C_n = \frac{1}{n+1}\binom{2n}{n} \approx \frac{1}{\sqrt{\pi}}\frac{4^n}{n^{3/2}} \quad \textit{\textbf{(large number for n big enough)}}$$

The catalan number has other forms:

$$C_n = \frac{1}{2n+1}\binom{2n+1}{n}, \\ = \binom{2n}{n} - \binom{2n}{n+1}.$$

The first Catalan numbers:

n	1	2	3	4	5	6	7	**8 (Decagon)**	9	10
C_n	1	2	5	14	42	132	429	**1 430**	4 862	16 796

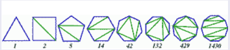


Figure: Number of triangulation of triangle (3 sides), square (4), pentagon (5), hexagon (6).

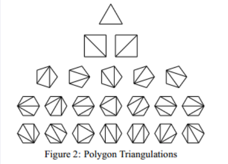


Figure: Polygon Triangulations.

There are of course many possible different triangulations of a given set of points

$\surd$

Figure: Left: Leonhard Euler (1707-1783) a Swiss mathematician. Right: Gabriel Lamé (1795-1870) was a French mathematician

Euler (1751): conjectured this result.
Goldbach and Segner (1758-1759): helped Euler complete the proof, in pieces.
Lamé (1838): first self-contained, complete proof.

The question now is what is the GOOD triangulation on a given set of points ?

But which triangulation?

The Answer Depends on the Method You Use...

For example in finite element methods, a triangulation is good if all triangles have large angles (large angles okay. Small angles bad.)

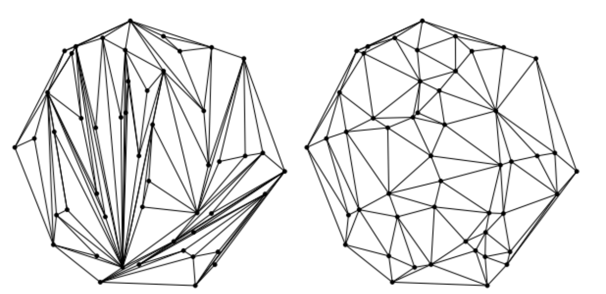


Figure: Two triangulations of the same set of 50 points.

Delaunay Triangulation (Boris N. Delaunay)

DT of a finite set of points P in $\mathbb{R}^d$ is a triangulation $DT(P)$ which satisfies the empty interior sphere condition. That is the circum-sphere of each simplex in $DT(P)$ does not contain any point of P in its interior.

Delaunay triangulation was introduced by Boris N. Delaunay (March 15, 1890 - July 17, 1980) in 1934 and is named in his honor.

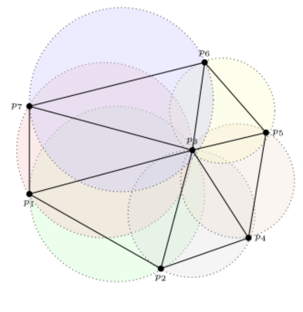


Figure: Boris N. Delaunay. Example of a Delaunay Triangulation

Example of DT

Let us have a set of 4 points in $\mathbb{R}^2$. We can create two triangulations on them.

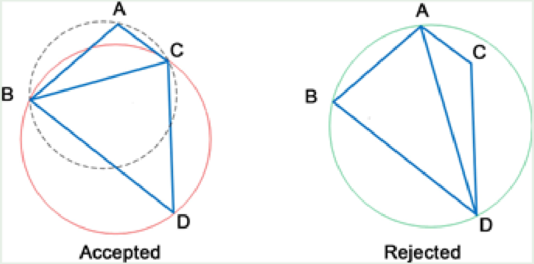


Figure: Example : 2 triangulations of the same set of 4 points.

- The triangulation on the right is any triangulation.
- The triangulation on the the lift is a DT, it satisfies the empty interior sphere condition.

What about existence of DT?

Theorem

DT of a set of points in $\mathbb{R}^d$ *always exists.*

What about Uniqueness of DT ?

Ingeneral,itisnotunique.

Theorem

a DT is unique if the set of points is in general position, i.e., no $d+2$ *points in* P *lie on a common sphere.*

DT of a human body.

We can create DT for domains with complex geometry. For example

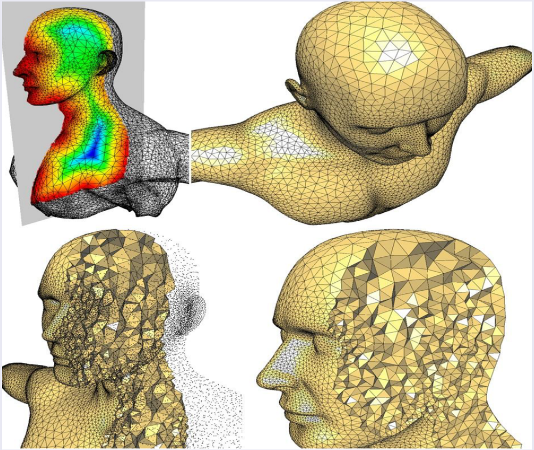


Figure: DT of a human body.

Optimal Properties of DT

In two dimensions:

- (1) The max-min angle property: DT maximizes the smallest angle: [Lawson 1977] and [Sibson 1978]

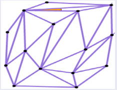


Figure: DT maximizes the smallest angle.

- (2) DT maximizes the arithmetic mean of the radius of inscribed circles of the triangles. Lambert (1994)
- (3) DT minimizes roughness (the integral of the squared gradients). Rippa (1990)
- (4)DT minimizes the maximum containing radius (the raduis of the smallest sphere containing the simplex). D'Azevedo and Simpson 1989. Rajan (1991) generalized this characterization to higher dimensions.

A Global Algorithm to Construct DT

1. Lift points to the parabolid
2. Form the lowest convex hull in $\mathbb{R}^{d+1}$
3. Project the lowest convex hull to $\mathbb{R}^d$

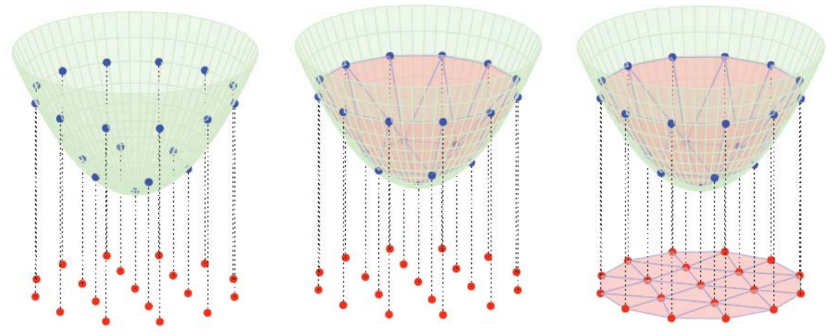
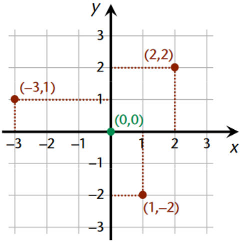
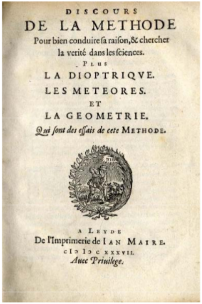


Figure: A Global Algorithm to Construct DT

Cartesian coordinates





René Descartes
(1596–1650)

Appendix "La Géométrie"
1637

Figure: Cartesian coordinates.

Barycentric coordinates

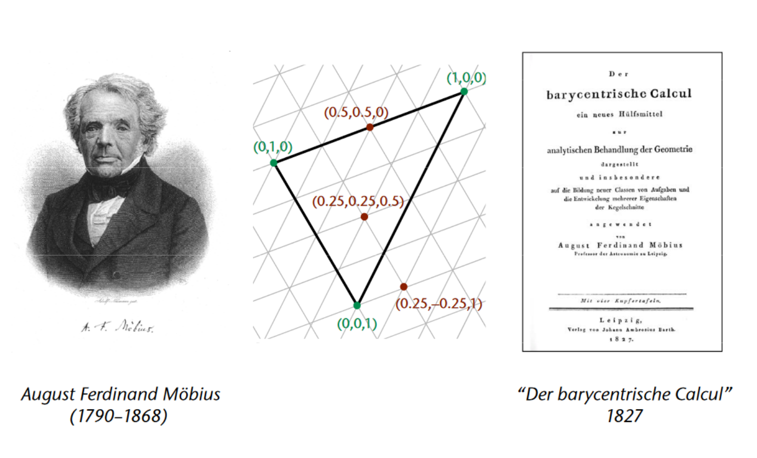


Figure: Barycentric coordinates.

Classical Barycentric coordinates

When dealing with a simplex it is often convenient to use barycentric coordinates. For all $\boldsymbol{x} \in \sigma^d = [\boldsymbol{v}_0 \boldsymbol{v}_1 \dots \boldsymbol{v}_d]$ and all $i = 0, \dots, d$, we denote by $\lambda_i(\boldsymbol{x})$ the components of vector $\boldsymbol{x} - \boldsymbol{v}_0$ in basis $\{\boldsymbol{v}_1 - \boldsymbol{v}_0, \dots, \boldsymbol{v}_d - \boldsymbol{v}_0\}$, i.e.

$$\boldsymbol{x} - \boldsymbol{v}_0 = \sum_{i=1}^{d} \lambda_i(\boldsymbol{x}) \left(\boldsymbol{v}_i - \boldsymbol{v}_0\right). \tag{3.1}$$

To allow all the vertices of σ^d to play a symmetric role, we introduce the additional function

$$\lambda_0(\boldsymbol{x}) := 1 - \sum_{i=1}^{d} \lambda_i(\boldsymbol{x}). \tag{3.2}$$

Classical Barycentric coordinates

A simple inspection of (3.1) and (3.2) reveals that coefficients $\lambda_i(\boldsymbol{x}),\ i = 0, \ldots, d$, are uniquely determined, they are affine functions of $\boldsymbol{x}$, and they satisfy the following three properties for a point $\boldsymbol{x}$ inside σ^d

$$\lambda_i(\boldsymbol{x}) \geq 0,\ i = 0, \ldots, d,\ \text{(positivity)} \tag{3.3}$$

$$1 = \sum_{i=0}^{d} \lambda_i(\boldsymbol{x}),\ \text{(partition of unity)} \tag{3.4}$$

$$\boldsymbol{x} = \sum_{i=0}^{d} \lambda_i(\boldsymbol{x})\boldsymbol{v}_i,\ \text{(linear precision).} \tag{3.5}$$

The uniquely determined coefficients $\lambda_i(\boldsymbol{x}), i = 0, \ldots, d$, are called the barycentric coordinates of $\boldsymbol{x}$ with respect to σ^d. Note that the linear precision (3.5) will continue to hold for any $\boldsymbol{x} \in \mathbb{R}^d$. However the positivity condition (3.3) is not satisfied in this case.

Barycentric coordinates for polygons

Let Ω be a convex polygon in $\mathbb{R}^2$ with vertices $\boldsymbol{v}_0, \ldots, \boldsymbol{v}_n$. Functions $\lambda_i : \Omega \to \mathbb{R}, i = 0, \ldots, n$ are called barycentric coordinates on Ω if they satisfy two properties:

- Non-negative on Ω: $\lambda_i(\boldsymbol{x}) \geq 0, \;\; i = 0, \ldots, n,$
- Partition of unity: $\sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) = 1,$
- Reproduces affine functions (linear precision): $\boldsymbol{x} = \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) \boldsymbol{v}_i.$ $(\forall \boldsymbol{x} \in \Omega)$

A general construction of barycentric coordinates over convex polygons. Many generalizations to choose from ...

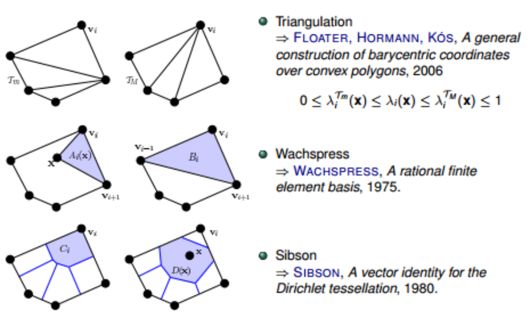


Figure: A general construction of barycentric coordinates over convex polygons.

Many generalizations to choose from ...

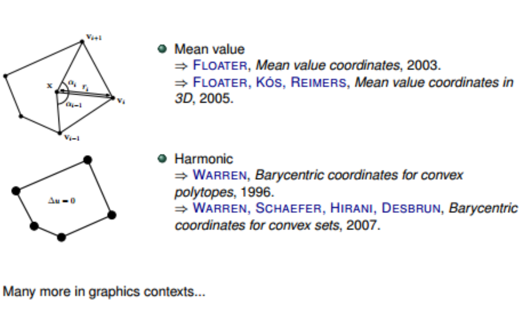


Figure: A general construction of barycentric coordinates over convex polygons.

Generalized Barycentric Coordinates in Convex polytopes

Given a point set $P := \{\boldsymbol{x}_i, i = 0, \ldots, n\} \subset \mathbb{R}^d$, denote by Ω be the convex hull of P. We define the notion of (generalized) barycentric coordinates as follows: let $\boldsymbol{x}$ be an arbitrary point of Ω. We call barycentric coordinates of $\boldsymbol{x}$ with respect to P any set of real coefficients $\{\lambda_i(\boldsymbol{x})\}_{i=0}^{n}$ depending on the points $\boldsymbol{x}_i$ of P and on $\boldsymbol{x}$ such that all the three following properties hold true:

- Convex combination: $\lambda_i(\boldsymbol{x}) \geq 0, \;\; i = 0, \ldots, n,$
- Partition of unity: $\sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) = 1,$
- Reproduces affine functions (linear completeness): $\boldsymbol{x} = \sum_{i=0}^{n} \lambda_i(\boldsymbol{x})\boldsymbol{x}_i$. $(\forall \boldsymbol{x} \in \Omega)$

Generalized Barycentric Coordinates for Convex polytopes

Recall that these coordinates exist for more general types of polytopes. The first result on their existence was due to Kalman (1961).

Theorem

Let $W = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_n\}$ *be a set of finite points of* $\mathbb{R}^d$ *and let the polytope* $\Omega = conv(W)$*. Then there exist nonnegative real-valued continuous functions* $\lambda_0, \lambda_1, \ldots, \lambda_n$ *defined on* Ω *such that*

$$\boldsymbol{x} = \sum_{i=0}^{n} \lambda_i(\boldsymbol{x})\boldsymbol{x}_i \quad \text{and} \quad \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) = 1 \tag{3.6}$$

for each $\boldsymbol{x} \in \Omega$.

Link between triangulations and barycentric coordinates

Every triangulation generates a set of barycentric coordinates : One possible natural approach for constructing an interesting class of particular barycentric coordinates would be to simply construct a triangulation of the polytope P the convex hull of the data set $P := \{\boldsymbol{x}_i, i = 0, \ldots, n\} \subset \mathbb{R}^d$ into simplices. We then use the standard barycentric coordinates for these simplices.

There are barycentric coordinates which are not generated by a triangulation

It should be noted that not every set of barycentric coordinates can be generated by a triangulation. Let $\Omega \subset \mathbb{R}^2$ be the rhombus shown and set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_4\}$. Then there are exactly two triangulations with respect to X: One $\mathcal{T}_1$ by connecting $\boldsymbol{x}_2$ with $\boldsymbol{x}_4$ and one $\mathcal{T}_2$ by connecting $\boldsymbol{x}_1$ with $\boldsymbol{x}_3$. The first one is a Delaunay triangulation. The second one is not a classical Delaunay triangulation. It should be noted that not every set of barycentric coordinates is generated by a triangulation. In fact, every convex combination of the barycentric coordinates with respect to the two triangulations generates a set of barycentric coordinates which are not generated by a triangulation.
We refer for details to:
A. Guessab, Generalized barycentric coordinates and approximations of convex functions on arbitrary convex polytopes, Computers and Mathematics with Applications 66 (2013). 1120-1136.

Barycentric Approximations

Given a point set $P := \{\boldsymbol{x}_i, i = 0, \ldots, n\} \subset \mathbb{R}^d$, denote by Ω be the convex hull of P and $\lambda(P) := \{\lambda_i, i = 0, \ldots, n\}$ a set of barycentric coordinates of P by using the points in P. Given a function $f : \Omega \to \mathbb{R}$, we define its barycentric approximation to be:

$$\boxed{B_n[f](\boldsymbol{x}) := \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) f(\boldsymbol{x}_i).}$$

The approximation operator B_n has many nice properties:

- Affine functions are exactly reproduced by B_n.
- It is widely used in computer graphics and geometric modeling, e.g. in Bézier and B-Spline techniques, linear finite element methods for simplicial meshes, Barycentric Finite Element Approximation.

Barycentric approximation based on triangulations

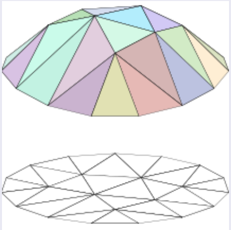


Figure: Barycentric approximation based on triangulations.

A characterization of the Delaunay triangulation

Here, we give a characterization of DT. Let $\mathcal{T}$ be a triangulation of Ω with respect to $X := \{\boldsymbol{x}_i, i = 0, \ldots, n\} \subset \mathbb{R}^d$ and let $\{\lambda_i, i = 0, \ldots, n\}$ be a set of barycentric coordinates with respect to $\mathcal{T}$.

Theorem

Triangulation $\mathcal{T}$ is a DT if and only if $B_n[\|.\|^2](\boldsymbol{x}) := \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) \|\boldsymbol{x}_i\|^2$ is a convex function on Ω.

Lipschitz continuous gradients

Notations: For any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$, we will denote the standard inner product of $\boldsymbol{x}$ and $\boldsymbol{y}$ by $\langle \boldsymbol{x}, \boldsymbol{y} \rangle$ and the Euclidean vector norm of $\boldsymbol{x} \in \mathbb{R}^d$ by $\|\boldsymbol{x}\| := \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$.
By $C^{1,1}(P)$ we denote the subclass of all functions f which are continuously differentiable on P with Lipschitz continuous gradients. This means that $f \in C^{1,1}(P)$, if there exists L_f such that for all $\boldsymbol{x}$ and $\boldsymbol{y}$ we have

$$\|\nabla f(\boldsymbol{y}) - \nabla f(\boldsymbol{x})\| \leq L_f \|\boldsymbol{y} - \boldsymbol{x}\| .$$

Characterization of all upper approximation operators

Theorem

Let $A : C^1(P) \to C(P)$ be a linear operator. The following statements are equivalent:

(i) *For every convex function $g \in C^{1,1}(P)$, we have*

$$g(\boldsymbol{x}) \leq A[g](\boldsymbol{x}), \ (\boldsymbol{x} \in P). \tag{5.1}$$

(ii) *For every $f \in C^{1,1}(P)$ with a Lipschitz constant gradient L_f, we have*

$$|f(\boldsymbol{x}) - A[f](\boldsymbol{x})| \leq \frac{L_f}{2} \left(A[\|.\|^2](\boldsymbol{x}) - \|\boldsymbol{x}\|^2 \right). \tag{5.2}$$

Equality is attained for all functions of the form

$$f(\boldsymbol{x}) = a(\boldsymbol{x}) + c\|\boldsymbol{x}\|^2, \tag{5.3}$$

where $c \in \mathbb{R}$ and $a(\cdot)$ is any affine function.

Applications to Barycentric Approximations

Corollary

Let B_n be the barycentric approximation given by

$$B_n[f](\boldsymbol{x}) = \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) f(\boldsymbol{x}_i). \tag{5.4}$$

Then for every function $f \in C^{1,1}(P)$ with a Lipschitz constant gradient L_f, we have

$$|f(\boldsymbol{x}) - B_n[f](\boldsymbol{x})| \leq \frac{L_f}{2}\left(B_n[\|.\|^2](\boldsymbol{x}) - \|\boldsymbol{x}\|^2\right). \tag{5.5}$$

Equality is attained for all functions of the form

$$f(\boldsymbol{x}) = a(\boldsymbol{x}) + c\|\boldsymbol{x}\|^2, \tag{5.6}$$

where $c \in \mathbb{R}$ and $a(\cdot)$ is any affine function.

Pointwise error estimations

For a function $f \in C^{1,1}(P)$, we denote

$$E_n[f](\boldsymbol{x}) \;:=\; E_n[f, \boldsymbol{\lambda}](\boldsymbol{x}) = \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) f(\boldsymbol{x}_i) - f(\boldsymbol{x}).$$

Pointwise error estimations

Lemma

The error $E_n[\|.\|^2]$ can be expressed in terms of the barycentric coordinates as:

$$E_n[\|.\|^2](\boldsymbol{x}) = \frac{1}{2}\sum_{i=0}^{n}\sum_{j=0}^{n}\lambda_i(\boldsymbol{x})\lambda_j(\boldsymbol{x})\,\|\boldsymbol{x}_i-\boldsymbol{x}_j\|^2 \quad (6.1)$$

$$= \sum_{i=0}^{n}\lambda_i(\boldsymbol{x})\,\|\boldsymbol{x}-\boldsymbol{x}_i\|^2 . \quad (6.2)$$

Now everything is set for giving an error estimate for convex functions with Lipschitz continuous gradients.

Theorem

For every function $f \in C^{1,1}(P)$ witha Lipschitz constant gradient L_f, we have

$$|E_n[f](\boldsymbol{x})| \leq \frac{L_f}{2} E_n[\|.\|^2](\boldsymbol{x}) \quad (6.3)$$

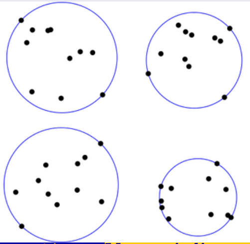
$$= \frac{L_f}{4} \sum_{i=0}^{n} \sum_{j=0}^{n} \lambda_i(\boldsymbol{x})\lambda_j(\boldsymbol{x}) \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2 \quad (6.4)$$

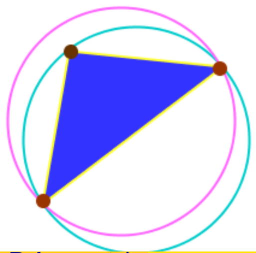
This inequality is sharp in the sense that the equality is attained for all affine functions.

smallest enclosing ball containing P

In this section we derive a practical error estimate, which will lead to a computationally attractive barycentric approximation. The error bound which is discussed in what follows, will be formulated in terms of the smallest enclosing ball containing P. We denote it by $SEB(P)$. $SEB(P)$ is the ball with the smallest radius which contains all the points in P. Let

$$SEB(P) := \left\{ \boldsymbol{x} \in \mathbb{R}^d : \left\| \boldsymbol{x} - \boldsymbol{c}^{\text{seb}} \right\| \leq r^{\text{seb}} \right\}.$$





A practical error bound

Theorem

For every function $f \in C^{1,r}(P)$ with a Lipschitz constant gradient L_f, we have

$$|E_n[f](\boldsymbol{x})| \leq \frac{L_f}{2}\left(\left(r^{seb}\right)^2 - \left\|\boldsymbol{x} - \boldsymbol{c}^{seb}\right\|^2\right), \quad (\boldsymbol{x} \in P). \tag{7.1}$$

This inequality is sharp in the sense that the equality is attained for all affine functions.

optimality of Delaunay triangulation

Now, in view of our error estimate, the following problem arises naturally:

Problem

Given a set of points, find the barycentric coordinates of the point set which provide the smallest error of the barycentric approximation of the quadratic function $\|.\|^2$.

optimality of Delaunay triangulation

Theorem

Let $T(P)$ be a triangulation of the point set X_n. Then the following statements are equivalent.

(i) *$T(P)$ is a Delaunay triangulation.*

(ii) *For any set of barycentric coordinates $\boldsymbol{\lambda} := \{\lambda_i\}_{i=0}^n$ and for all $\boldsymbol{x} \in P$, there holds*

$$0 \leq E_n^{T(P)}[\|.\|^2](\boldsymbol{x}) \leq E_n[\|.\|^2, \boldsymbol{\lambda}](\boldsymbol{x}).$$

Numerical experiments

Given a set of scattered data $\{(x_i, y_i, f_i\}_{i=1}^{N}$, which are assumed to be sampled from a convex function $f : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$. Taking the N scattered points as nodes, an optimal triangulation mesh, T, is constructed in domain Ω using Delaunay triangulation. In this section, we present two numerical examples which illustrate the proposed methodology. We approximate two test convex functions using randomly scattered data points in the indicated domain.

Numerical experiments

Example

We take the following convex function $f(x, y) := 500\exp((x-0.5)^2 + (y-0.5)^2)$, with the restriction of domain $D := [0,1] \times [0,1]$. The data is generated from the above function and it is based on 21 equally spaced nodes on each edge of the boundary of square D and 216 nodes in the square D. The nodes in the domain are placed randomly selected from D while the nodes on the boundary is equally spaced.

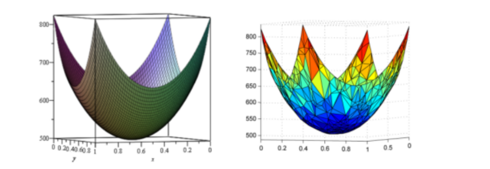


Figure: The figure on the left shows the graph of f and the graph on the right for the linear interpolation of the data generated from f.

Numerical experiments

Example

In the second example the data points is generated from the following test function $g(x,y) = x^3 + 5(y^2 - 0.6)^2 + 1$, with the restriction of domain $D := [0,1] \times [0,1]$. As it is mentioned, the data points in this example belong to a surface that models part of a car. The Nodes are randomly selected as in example below.

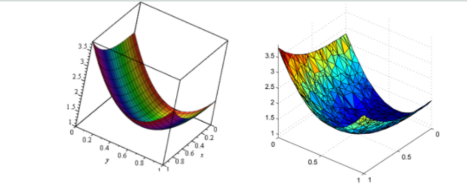


Figure: The figure on the left shows the graph of g and the graph on the right for the linear interpolation of the data generated from g.

Negative *definite cubature formula*

Given a point set $P := \{\boldsymbol{x}_i, i = 1, \ldots, n\} \subset \mathbb{R}^d$, denote by Ω be the convex hull of P.

Definition

For n points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \Omega$, called *nodes*, and associated positive numbers $A_1, \ldots, A_n$, we say that

$$\{(A_i, \boldsymbol{x}_i) \ : \ i = 1, \ldots, n\} \tag{10.1}$$

defines the negative *definite cubature formula* (nd formula)

$$\int_\Omega f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \sum_{i=1}^{n} A_i f(\boldsymbol{x}_i) + R_n[f] \tag{10.2}$$

if the approximation error $R_n[f] \le 0$ for all convex functions $f \in C(\Omega)$. ($\Rightarrow$ $nd-$formula approximates from above the exact value of the integral of any continuous convex functions)

First characterization of nd-formulas in terms of the approximation error

Theorem

Let $\Omega \subset \mathbb{R}^d$ be a compact convex set. A cubature formula is nd-formula if and only if for all $f \in C^2(\Omega)$, we have

$$|R_n[f]| \leq \left|R_n\left[\|\cdot\|^2\right]\right| \cdot \frac{\left|D^2 f\right|}{2}. \tag{10.3}$$

In (10.3), equality is attained for all functions of the form

$$f(\boldsymbol{x}) := a(\boldsymbol{x}) + c\|\boldsymbol{x}\|^2,$$

where $c \in \mathbb{R}$ and $a(\cdot)$ is any affine function.

Allal Guessab Gerhard Schmeisser, Negative Definite Cubature Formulas, Extremality and Delaunay Triangulation, Constr Approx (2010) 31: 95-113.

PARTITIONS OF UNITY

Let $\Omega \subset \mathbb{R}^d$ be a compact convex polytope. We say that a system $\{\phi_1, \dots, \phi_n\}$ of real-valued functions is a *partition of unity* on Ω if:

(i) $\phi_i \in L^1(\Omega)$ and $\int_\Omega \phi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} > 0$ for $i = 1, \dots, n$;

(ii) $\phi_i(\boldsymbol{x}) \geq 0$ a. e. on Ω for $i = 1, \dots, n$;

(iii) $\phi_1(\boldsymbol{x}) + \cdots + \phi_n(\boldsymbol{x}) = 1$ a. e. on Ω.

Second haracterization of nd-formulas in terms of PU

Now we can characterize nd-formulas as follows.

Theorem

A set $\mathfrak{a} = \{(A_i, \boldsymbol{x}_i) : i = 1, \dots, n\}$ *defines a nd−formula on* Ω *if and only if there exists a partition of unity* $\{\phi_1, \dots, \phi_n\}$ *on* Ω *such that*

$$\boldsymbol{x} = \sum_{i=1}^{n} \phi_i(\boldsymbol{x})\boldsymbol{x}_i \qquad (a.\ e.\ on\ \Omega) \tag{10.4}$$

and

$$A_i := \int_\Omega \phi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \qquad (i = 1, \dots, n). \tag{10.5}$$

Guessab, Allal; Schmeisser, Gerhard: Construction of positive definite cubature formulas and approximation of functions via Voronoi tessellations. Adv. Comput. Math. 32 (2010), no. 1, 25-41.

Minimal negative definite cubature formulas

In order to select good nd-formulas, we define a preorder on the set of nd-formulas.

Definition

For two nd-formulas

$$\mathfrak{a} := \sum_{i=1}^{n} a_i f(\boldsymbol{x}_i) \quad \text{and} \quad \mathfrak{b} := \sum_{j=1}^{m} b_j f(\boldsymbol{y}_j), \tag{10.6}$$

we write $\mathfrak{b} \prec \mathfrak{a}$
if

$$\sum_{j=1}^{m} B_j f(\boldsymbol{y}_j) \leq \sum_{i=1}^{n} A_i f(\boldsymbol{x}_i), \tag{10.7}$$

for every convex function $f \in C(\Omega)$. We say that an nd-formula $\mathfrak{a}$ with n nodes defines a *minimal* nd-formula if there is no nd-formula $\mathfrak{b}$ with n nodes such that $\mathfrak{b} \prec \mathfrak{a}$ and $\mathfrak{b} \neq \mathfrak{a}$.

Extension of Delaunay Triangulation

In order to determine minimal nd-formulas, we give another characterization of DT. Let $\mathcal{T}$ be a triangulation of Ω with respect to X and let $g(\boldsymbol{x}) := \|\boldsymbol{x}\|^2$. Denote by $B_n[\|.\|^2](\boldsymbol{x}) := \sum_{i=0}^{n} \lambda_i(\boldsymbol{x}) \|\boldsymbol{x}_i\|^2$

Theorem

Triangulation $\mathcal{T}$ is a DT if and only if $B_n[\|.\|^2](\boldsymbol{x})$ is a convex function on Ω.

Now, let g any continuous convex function. If $B_n[g](\boldsymbol{x})$ is convex then we call $\mathcal{T}$ a DT with respect to X and g.

Minimal nd-formulas

Theorem

Let $g \in C(\Omega)$ be a strictly convex function and let $\mathcal{T}$ be a DT with respect to X and g. Then the cubature formula obtained by integrating $B_n[g]$ is a minimal nd-formula.

Theorem

Every nd-formula which only has vertices of Ω as nodes is minimal.

Optimal negative definite cubature formulas

The error estimate of every nd-formula satisfies

$$|R_n[f]| \leq \left|R_n\left[\|\cdot\|^2\right]\right| \cdot \frac{\left|D^2 f\right|}{2} \tag{10.8}$$

then it is interesting to select nd-formulas for which $\left|R_n[\|\cdot\|^2]\right|$ is small.

$\left|R_n[\|\cdot\|^2]\right| \to \min$ **among all nd-formulas with n nodes**

Definition

We say that a nd-formula is optimal if among all nd-formulas with n nodes, $\left|R_n[\|\cdot\|^2]\right|$ attains a smallest value.

Optimal Cubature formulas

Theorem

Let $\mathcal{T}$ be a DT with respect to X. Then the cubature formula obtained by integrating $B_n[g]$ is an optimal nd-formula for X.

Voronoi Tessellations

1. Given
   - a subset $\Omega \subset \mathbb{R}^d$ and a set $X = \{\boldsymbol{x}_i\}_{i=1}^{n} \subset \Omega$
   - a distance function $d(.,.)$ defined for Ω and X
2. Then, the Voronoi subset or Voronoi region $V_i \subset \Omega$ is the set of all points in Ω that are closer to $\boldsymbol{x}_i$ than to all other points of X, that is,
$$V_i = \{\boldsymbol{x} \in \Omega : d(\boldsymbol{x}, \boldsymbol{x}_i) \leq d(\boldsymbol{x}, \boldsymbol{x}_j), j = 1, \ldots, n\} \tag{11.1}$$
3. We call the set of Voronoi subsets $\{V_1, V_2, \ldots, V_n\}$ a Voronoi tessellation of Ω with respect to the given set of generators X

Figure: Georgi Voronoi

Centroidal Voronoi Tessellations

A Centroidal Voronoi Tessellation (CVT) is a Voronoi tessellation where each generator $\boldsymbol{x}_i$ coincides with the center of gravity of each Voronoi region V_i, that is:

$$\boldsymbol{x}_i = \boldsymbol{x}_i^* = \frac{\int_{V_i} \boldsymbol{x} d\boldsymbol{x}}{\int_{V_i} d\boldsymbol{x}}, i = 1, \ldots, n. \tag{11.2}$$

Centroidal Voronoi Tessellations

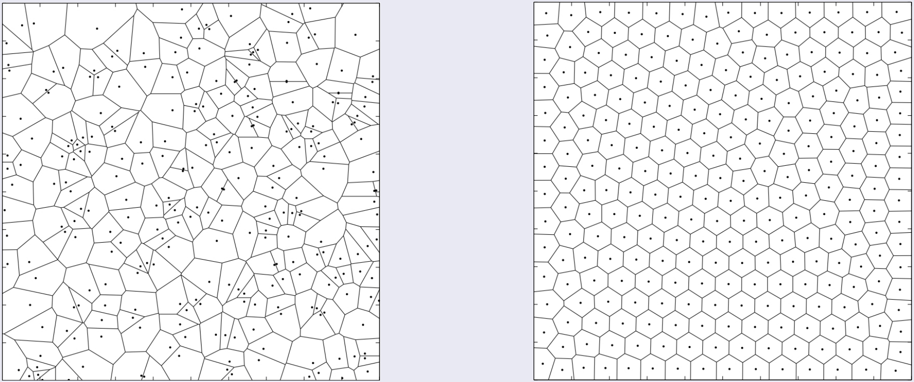


Figure: Left: the Voronoi tessellation of 256 uniformly distributed randomly selected points in the square. Right: a 256-point CVT of the square corresponding to a uniform density

An example of CVT in the case of a complex geometry domain

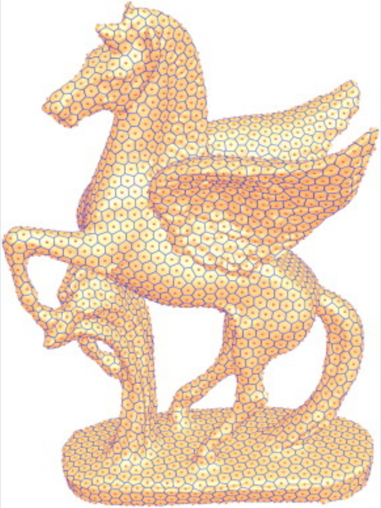
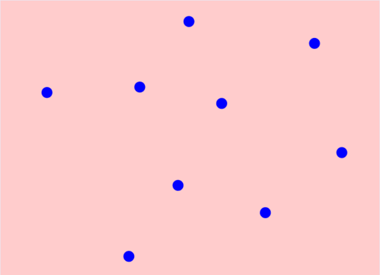


Figure: An example of a complex geometry domain

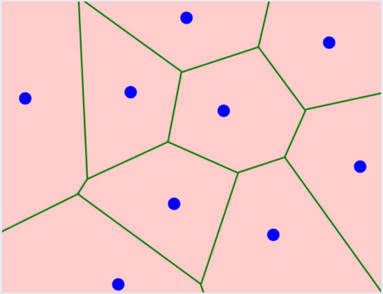
Link between Voronoi diagram and Delaunay Triangulation

Let $P = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ a set of n points in the plane.



Link between Voronoi diagram and Delaunay Triangulation

Let $P = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ a set of n points in the plane.



Link between Voronoi diagram and Delaunay Triangulation

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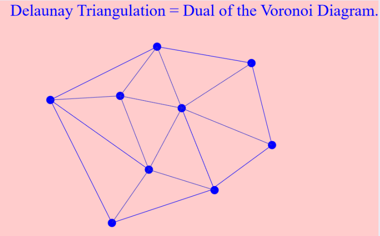
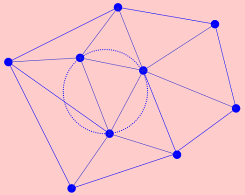


Link between Voronoi diagram and Delaunay Triangulation

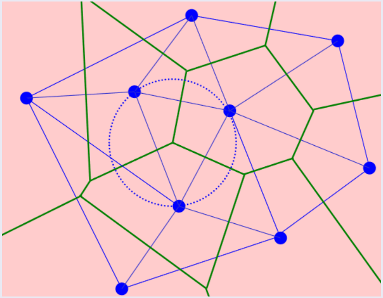
Let $P = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ a set of n points in the plane.



Delaunay triangles have the “empty circle” property.

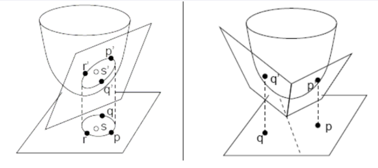
Link between Voronoi diagram and Delaunay Triangulation

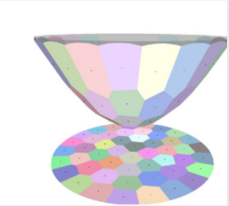
Let $P = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ a set of n points in the plane.



Voronoi diagram: A different Formulation

Let $P = \{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}$ a set of n points in $\mathbb{R}^d$





- Project each point $\boldsymbol{p}_i$ on the surface of a unit paraboloid
- Draw tangent planes of the paraboloid at every projected point.
- Compute the upper envelope of these hyperplanes.

Result: The projection of this upper envelope gives the Voronoi diagram of the point set.

Positive *definite cubature formula*

Given a point set $P := \{\boldsymbol{x}_i, i = 1, \ldots, n\} \subset \mathbb{R}^d$, denote by Ω be the convex hull of P.

Definition

For n points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \Omega$, called *nodes*, and associated positive numbers $A_1, \ldots, A_n$, we say that

$$\big\{(A_i, \boldsymbol{x}_i) \;:\; i = 1, \ldots, n\big\} \tag{12.1}$$

defines the positive *definite cubature formula* (pd-formula)

$$\int_\Omega f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} = \sum_{i=1}^{n} A_i f(\boldsymbol{x}_i) + R_n[f] \tag{12.2}$$

if $R_n[f] \geq 0$ for all convex functions $f \in C(\Omega)$.
($\Rrightarrow$ *pd*−formula approximates from below the exact value of the integral of any continuous convex functions.)

differences between nd and pd-formulas

There is not much analogy between nd and pd-formulas. pd-formulas exist for all compact convex sets , however the existence of an nd-formula requires to be a convex polytope whose vertices are among the nodes.

First characterization of positive definite cubature formulas

An interesting characterization of pd-formulas is provided by the following statement Theorem.

Theorem

Let $\Omega \subset \mathbb{R}^d$ be a compact convex set. A cubature formula is pd if and only if for all $f \in C^2(\Omega)$, we have

$$|R_n[f]| \leq \left|R_n\left[\|\cdot\|^2\right]\right| \cdot \frac{\left|D^2 f\right|}{2}. \tag{12.3}$$

In (12.3), equality is attained for all functions of the form

$$f(\boldsymbol{x}) := a(\boldsymbol{x}) + c\|\boldsymbol{x}\|^2,$$

where $c \in \mathbb{R}$ and $a(\cdot)$ is any affine function.

Allal Guessab Gerhard Schmeisser: Construction of positive definite cubature formulas and approximation of functions via Voronoi tessellations. Adv. Comput. Math. 32 (2010), no. 1, 25-41.

Second characterization of pd-formulas

Now we can characterize pd-formulas as follows.

Theorem

(Allal Guessab Gerhard Schmeisser, 2010)
A set $\mathfrak{a} = \{(A_i, \boldsymbol{x}_i) : i = 1, \ldots, n\}$ *defines a pd-formula on* Ω *if and only if there exists a partition of unity* $\{\phi_1, \ldots, \phi_n\}$ *on* Ω *such that*

$$\boldsymbol{x}_i := \int_\Omega \boldsymbol{x}\phi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \qquad (i = 1, \ldots, n), \tag{12.4}$$

and

$$A_i := \int_\Omega \phi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \qquad (i = 1, \ldots, n). \tag{12.5}$$

Maximal positive definite cubature formulas

In order to select good pd-formulas, we define a preorder on the set of pd-formulas.

Definition

For two pd-formulas

$$\mathfrak{a} := \sum_{i=1}^{n} a_i f(\boldsymbol{x}_i) \quad \text{and} \quad \mathfrak{b} := \sum_{j=1}^{m} b_j f(\boldsymbol{y}_j), \tag{12.6}$$

we write $\mathfrak{b} \prec \mathfrak{a}$
if

$$\sum_{j=1}^{m} B_j f(\boldsymbol{y}_j) \leq \sum_{i=1}^{n} A_i f(\boldsymbol{x}_i), \tag{12.7}$$

for every convex function $f \in C(\Omega)$. We say that an pd-formula $\mathfrak{a}$ of length n defines a *maximal* pd-formula if there is no pd-formula $\mathfrak{b}$ with n terms such that $\mathfrak{a} \prec \mathfrak{b}$ and $\mathfrak{a} \neq \mathfrak{b}$.

optimal pd- formulas

In view of the error estimates

$$|R_n[f]| \leq \left|R_n\left[\|\cdot\|^2\right]\right| \cdot \frac{\left|D^2 f\right|}{2}. \tag{12.8}$$

it seems desirable to select nd-formulas for which $\left|R_n[\|\cdot\|^2]\right|$ is small.

Definition

We say that a pd-formula is optimal if among all pd-formulas with n nodes, $\left|R_n[\|\cdot\|^2]\right|$ attains a smallest value.

$$\left|R_n[\|\cdot\|^2]\right| \rightarrow \min \text{ among all pd-formulas with n nodes}$$

Optimality of pd-formulas implies maximality

Theorem

Each optimal pd-formula is maximal.

(Guessab, Allal; Nouisser, Otheman; Schmeisser, Gerhard: A definiteness theory for cubature formulas of order two. Constr. Approx. 24 (2006), no. 3, 263-288

Extremal properties of centroidal Voronoi tessellations

Centroidal Voronoi tessellations always generate pd-formulas. But they can also generate “good” pd-formulas.

Theorem

Every optimal pd-formula can be generated by a CVT.

The converse the above Theorem is not true. Does the pd-formula generated by any centroidal Voronoi tessellation always have a certain extremal property?

Theorem

Every CVT generates a maximal pd-formula.

Numerical experiments in 3D

We have chosen the following exponential of an affine function as test function $g(x, y, z) = \exp(ax + by + cz)$, and the domain of integration is the pyramid

$$Pyr = \{(x, y; z) \in \mathbb{R}^3 : 0.3z < x < 1 - 0.3z, 0.3z < y < 1 - 0.3z, 0 < z < 1\}.$$

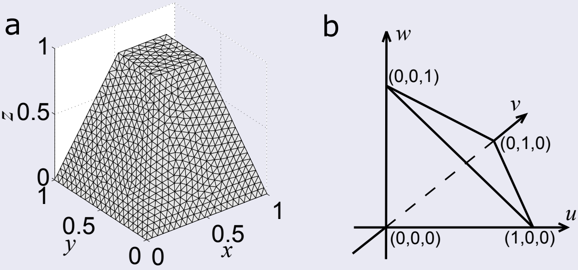


Figure: (a) Domain of the pyramid and its decomposition into tetrahedra generated by DistMesh. (b) Reference tetrahedron.

Numerical examples in 3D

The exact value was obtained using Mathematica.

$$\begin{aligned} I_{pyr}(g) &= K(Aa^3 + Ba^2b + Ca^2c + Db^2a + Eb^2c + Fb^3 + Gc^3 + Hc^2a \\ &+ Ic^2b + Jabc) \end{aligned}$$

$K = \dfrac{10}{ab(3a-3b-10c)(3a+3b-10c)(3a-3b+10c)(3a+3b+10c)}$,
$A = 27(e^b - e^a + e^{a+b} + \alpha + \beta - \gamma - \theta - 1)$,
$B = 27(e^b - e^a - e^{a+b} - \alpha + \beta - \gamma + \theta + 1)$,
$C = 90(e^{a+b} - e^a - e^b - \alpha + \beta + \gamma - \theta + 1)$,
$D = 27(e^a - e^b - e^{a+b} - \alpha - \beta + \gamma + \theta + 1)$,
$E = 90(-e^a - e^b + e^{a+b} - \alpha + \beta + \gamma - \theta + 1)$,
$F = 27(e^a - e^b + e^{a+b} + \alpha - \beta + \gamma - \theta - 1)$,
$G = 1000(e^a + e^b - e^{a+b} + \alpha - \beta - \gamma + \theta - 1)$,
$H = 300(e^a - e^b - e^{a+b} - \alpha - \beta + \gamma + \theta + 1)$,
$I = 300(e^b - e^a - e^{a+b} - \alpha + \beta - \gamma + \theta + 1)$,
$J = 180(-e^a - e^b - e^{a+b} + \alpha + \beta + \gamma + \theta - 1)$,
$\alpha = e^{0.3a+0.3b+c}$, $\beta = e^{0.7a+0.3b+c}$, $\gamma = e^{0.3a+0.7b+c}$, $\theta = e^{0.7a+0.7b+c}$.

Numerical examples in 3D

Table: Errors obtained while integrating g with $a = 1$, $b = 2$, $c = 3$ over pyramid Pyr

	Relative errors of integration		
N	$E_N^{\mathrm{CVT}}(g)$	$E_N^{\mathrm{DEL}}(g)$	
4	1.365E-02	-6.777E-03	
8	2.992E-03	-1.494E-03	
16	6.990E-04	-3.494E-04	
32	1.629E-04	-8.142E-05	
64	3.959E-05	-1.979E-05	
128	8.725E-06	-6.171E-06	

Somme Papers

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