Mathematical definitions for PyTelTools

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1 Introduction

We call informally a **2D mesh** \mathcal{M} , or simple **mesh**, a finite network where

- an **element** \mathcal{T} is a triangle in \mathbb{R}^2 ; we write $\mathcal{T} \in \mathcal{M}$; its vertices $P_{1,2,3}$ are called **points** of the mesh;
- a **connection** is an common edge (two common vertices) between two elements; such that
 - every two elements can either intersect at one common vertex, intersect at one common edge (two common vertices), or have empty intersection;
 - every element has at least one common edge with another element (the mesh is **connected**).

Furthermore, for some integer t between 0 and T_{max} , a mesh can have a **valuation** \mathcal{V}_t at time t, which assigns to each point of the mesh a real number, called the **value** of the point.

Other useful notations include

- area (\mathcal{T}) is the area of the triangle \mathcal{T} ;
- area $(\mathcal{M}) = \sum_{\mathcal{T} \in \mathcal{M}} \operatorname{area}(\mathcal{T})$ is the total area of elements in the mesh \mathcal{M} ;
- size(\mathcal{M}) is the number of elements in the mesh \mathcal{M} .

2 Interpolation

Definition 1. Let \mathcal{T} be a triangle in \mathbb{R}^2 of vertices $P_{1,2,3}$, for a point $Q \in \mathcal{T}$ (in the interior or on the boundary), the **barycentric coordinates** of Q is equal to

$$\lambda_1 = \frac{\operatorname{area}(\mathcal{T}_1)}{\operatorname{area}(\mathcal{T})}, \quad \lambda_2 = \frac{\operatorname{area}(\mathcal{T}_2)}{\operatorname{area}(\mathcal{T})}, \quad \lambda_3 = \frac{\operatorname{area}(\mathcal{T}_3)}{\operatorname{area}(\mathcal{T})}$$

where \mathcal{T}_1 , \mathcal{T}_2 , \mathcal{T}_3 are triangles in \mathbb{R}^2 defined by the vertices $P_2 P_3 Q$, $P_1 P_3 Q$ and $P_1 P_2 Q$ (when Q is on the boundary of \mathcal{T} , one or two of the triangles \mathcal{T}_1 , \mathcal{T}_2 , \mathcal{T}_3 are considered to be empty triangle).

Definition 2. Given a mesh \mathcal{M} valuated at \mathcal{V}_t and an element $\mathcal{T} \in \mathcal{M}$ of vertices $P_{1,2,3}$, the **interpolated** value of a point $Q \in \mathcal{T}$ is equal to the dot product of the barycentric coordinates of Q and the values of $P_{1,2,3}$:

$$\lambda_1 \mathcal{V}_t(P_1) + \lambda_2 \mathcal{V}_t(P_2) + \lambda_3 \mathcal{V}_t(P_3)$$

3 Sub-triangulation

3.1 Definition

Definition 3. A sub-triangulation $(\mathcal{M}^*, \mathcal{V}_t^*)$ of a mesh \mathcal{M} valuated at \mathcal{V}_t is the result of the operation that, for every element $\mathcal{T} \in \mathcal{M}$ of vertices $P_{1,2,3}$,

- adds a point Q in the interior of \mathcal{T} and splits \mathcal{T} into three elements \mathcal{T}_1 , \mathcal{T}_2 , \mathcal{T}_3 of vertices $P_2 P_3 Q$, $P_1 P_3 Q$ and $P_1 P_2 Q$, called the splits of \mathcal{T} at Q;
- extends \mathcal{V}_t to Q and assigns to Q the interpolated value at Q.

We note $ST(\mathcal{M}, \mathcal{V}_t)$ the set of all sub-triangulations of \mathcal{M} valuated at \mathcal{V}_t .

3.2 Invariance under sub-triangulation

Definition 4. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , a function f of $(\mathcal{M}, \mathcal{V}_t)$ is **invariant under subtriangulation** if f is constant in the set of all sub-triangulations of \mathcal{M} valuated at \mathcal{V}_t :

$$\forall (\mathcal{M}^*, \mathcal{V}_t^*) \in \mathrm{ST}(\mathcal{M}, \mathcal{V}_t), \quad f(\mathcal{M}^*, \mathcal{V}_t^*) = f(\mathcal{M}, \mathcal{V}_t).$$

4 Flux

TODO: coming soon

Define mass flux

Define simplified fluxes:

— line flux

— area flux

5 Volume

5.1 Volume of an element

Definition 5. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , the **volume** volume $_t(\mathcal{T}, \mathcal{V}_t)$ **of an element** $\mathcal{T} \in \mathcal{M}$ (also called **net volume**) of vertices $P_{1,2,3}$ is the product of the area of \mathcal{T} by one third the sum of the values of its three vertices:

volume $_t(\mathcal{T}, \mathcal{V}_t) = \frac{\operatorname{area}(\mathcal{T})}{3} \sum_{P_i} \mathcal{V}_t(P_i).$

5.2 Explanation

The definition of the volume of an element \mathcal{T} valuated at \mathcal{V}_t can be easily understood by picturing the **truncated right triangular prism** $\overline{\mathcal{T}}_t$ in \mathbb{R}^3 naturally induced by the valuation \mathcal{V}_t .

If we note (x_1, y_1) , (x_2, y_2) , (x_3, y_3) the coordinates of the three vertices $P_{1,2,3}$ of \mathcal{T} in a Cartesian coordinate system, then the prism $\overline{\mathcal{T}}_t$ is defined by the following six vertices (figure 1):

- the **projected points** $\overline{P}_{1,2,3}$ of coordinates $(x_1, y_1, 0), (x_2, y_2, 0), (x_3, y_3, 0)$ which form the **base** triangle of the prism,
- the **valuated points** $\overline{P}_{1,2,3}^{\mathcal{V}_t}$ of coordinates $(x_1, y_1, \mathcal{V}_t(P_1)), (x_2, y_2, \mathcal{V}_t(P_2)), (x_3, y_3, \mathcal{V}_t(P_3))$ which form the **upper triangle** of the prism.

This prism is truncated because the upper triangle is not necessarily parallel to the base triangle; it is also a right prism because the three lateral edges is always perpendicular to the base triangle.

It is known from the classical geometry that the volume of a truncated right triangular prism is equal to the product of its base by one third the sum of its lateral edges. The volume of an element \mathcal{T} valuated at \mathcal{V}_t in definition 5 corresponds thus to the volume of its induced prism.

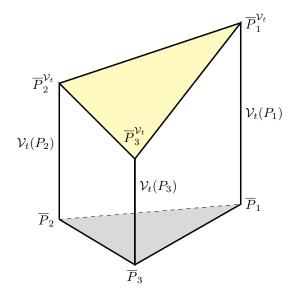


FIGURE 1 – The induced prism $\overline{\mathcal{T}}_t$ of an element \mathcal{T} valuated at \mathcal{V}_t

Since the valuation V_t can take positive and negative values, the upper triangle does not always lie on the half-space z > 0 or z < 0. When the upper triangle intersects the base triangle, the induced prism $\overline{\mathcal{T}}_t$ is not a polyhedron, but the volume defined above is still valid.

5.3 Volume of a mesh

Definition 6. The volume volume $_t^{abs}(\mathcal{M}, \mathcal{V}_t)$ of a mesh \mathcal{M} valuated at \mathcal{V}_t is the sum of the volumes of its elements:

$$\mathrm{volume}_{t}(\mathcal{M},\,\mathcal{V}_{t}) = \sum_{\mathcal{T} \in \mathcal{M}} \mathrm{volume}_{t}(\mathcal{T},\,\mathcal{V}_{t}).$$

Proposition 1. The volume of a mesh \mathcal{M} valuated at \mathcal{V}_t defined in definition 6 is invariant under subtriangulation.

Proof. Let \mathcal{M} be a mesh valuated at \mathcal{V}_t and $(\mathcal{M}^*, \mathcal{V}_t^*) \in ST(\mathcal{M}, \mathcal{V}_t)$. Let \mathcal{T} be any element of \mathcal{M} and $\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3$ its splits in \mathcal{M}^* at the point Q. First we write down the total volume of the three splits:

$$\sum_{k=1}^{3} \text{volume}_{t}(\mathcal{T}_{k}, \mathcal{V}_{t}^{*})
= \frac{\text{area}(\mathcal{T}_{1})}{3} (\mathcal{V}_{t}^{*}(P_{2}) + \mathcal{V}_{t}^{*}(P_{3}) + \mathcal{V}_{t}^{*}(Q)) + \frac{\text{area}(\mathcal{T}_{2})}{3} (\mathcal{V}_{t}^{*}(P_{1}) + \mathcal{V}_{t}^{*}(P_{3}) + \mathcal{V}_{t}^{*}(Q))
+ \frac{\text{area}(\mathcal{T}_{3})}{3} (\mathcal{V}_{t}^{*}(P_{1}) + \mathcal{V}_{t}^{*}(P_{2}) + \mathcal{V}_{t}^{*}(Q))
= \frac{1}{3} \sum_{k=1}^{3} \left(\mathcal{V}_{t}^{*}(P_{k}) \sum_{\substack{j=1,2,3\\j\neq k}} \text{area}(\mathcal{T}_{j}) \right) + \frac{1}{3} \mathcal{V}_{t}^{*}(Q) \sum_{k=1}^{3} \text{area}(\mathcal{T}_{k}).$$

By the definition of sub-triangulation, the values $\mathcal{V}_t^*(P_k) = \mathcal{V}_t(P_k)$ and the value of Q is equal to

$$\mathcal{V}_t^*(Q) = \sum_{k=1}^3 \lambda_k \, \mathcal{V}_t(P_k) = \frac{1}{\operatorname{area}(\mathcal{T})} \sum_{k=1}^3 \operatorname{area}(\mathcal{T}_k) \, \mathcal{V}_t(P_k) = \frac{\sum_{k=1}^3 \operatorname{area}(\mathcal{T}_k) \, \mathcal{V}_t(P_k)}{\sum_{k=1}^3 \operatorname{area}(\mathcal{T}_k)},$$

thus,

$$\sum_{k=1}^{3} \text{volume}_{t}(\mathcal{T}_{k}, \mathcal{V}_{t}^{*}) = \frac{1}{3} \sum_{k=1}^{3} \left(\mathcal{V}_{t}(P_{k}) \sum_{\substack{j=1,2,3 \\ j \neq k}} \text{area}(\mathcal{T}_{j}) \right) + \frac{1}{3} \sum_{k=1}^{3} \text{area}(\mathcal{T}_{k}) \mathcal{V}_{t}(P_{k})$$

$$= \frac{1}{3} \sum_{k=1}^{3} \left(\mathcal{V}_{t}(P_{k}) \sum_{j=1}^{3} \text{area}(\mathcal{T}_{j}) \right) = \frac{\text{area}(\mathcal{T})}{3} \sum_{k=1}^{3} \mathcal{V}_{t}(P_{i})$$

$$= \text{volume}_{t}(\mathcal{T}, \mathcal{V}_{t}).$$

Therefore,

$$\operatorname{volume}_{t}(\mathcal{M}^{*}, \mathcal{V}_{t}^{*}) = \sum_{\mathcal{T} \in \mathcal{M}} \left(\sum_{\substack{\mathcal{T}_{k} \\ \text{splits of } \mathcal{T}}} \operatorname{volume}_{t}(\mathcal{T}_{k}, \mathcal{V}_{t}^{*}) \right) = \sum_{\mathcal{T} \in \mathcal{M}} \operatorname{volume}_{t}(\mathcal{T}, \mathcal{V}_{t}) = \operatorname{volume}_{t}(\mathcal{M}, \mathcal{V}_{t}).$$

5.4 Positive and negative volumes of an element

Definition 7. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , the **positive volume** volume $_t^+(\mathcal{T}, \mathcal{V}_t)$ of an element $\mathcal{T} \in \mathcal{M}$ of vertices $P_{1,2,3}$, is equal to

- 0, if $V_t(P_i) \leq 0$ for i = 1, 2, 3 (the upper triangle lies in the half-space $z \leq 0$);
- its net volume volume $_t(\mathcal{T}, \mathcal{V}_t)$, if $\mathcal{V}_t(P_i) \ge 0$ for i = 1, 2, 3 (the upper triangle lies in the half-space $z \ge 0$);
- otherwise, the upper triangle intersect the plane z=0 at a segment $Q_1 Q_2$ (figure 2). There are two cases:
 - if \mathcal{T} has only one vertex, w.l.o.g. P_1 , such that $\mathcal{V}_t(P_1) > 0$, the positive volume is equal to the volume of the tetrahedron defined by Q_1 , Q_2 , the projected point \overline{P}_1 and the valuated point $\overline{P}_1^{\mathcal{V}_t}$ of P_1 ;
 - otherwise, \mathcal{T} has only one vertex, w.l.o.g. P_1 , such that $\mathcal{V}_t(P_1) < 0$. The positive volume is equal to the difference between the net volume volume $t(\mathcal{T}, \mathcal{V}_t)$ and the volume of the tetrahedron defined by Q_1 , Q_2 , the projected point \overline{P}_1 and the valuated point $\overline{P}_1^{\mathcal{V}_t}$ of P_1 .

Definition 8. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , the **negative volume** volume $_t^-(\mathcal{T}, \mathcal{V}_t)$ of an element $\mathcal{T} \in \mathcal{M}$ is equal to the difference between its net volume and its positive volume:

$$volume_t^-(\mathcal{T}, \mathcal{V}_t) = volume_t(\mathcal{T}, \mathcal{V}_t) - volume_t^+(\mathcal{T}, \mathcal{V}_t).$$

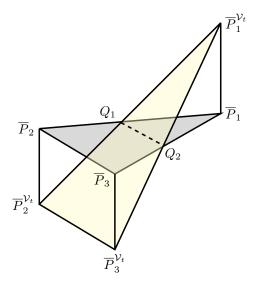


Figure 2 – When the upper triangle intersects the base triangle at a segment $Q_1 Q_2$

5.5 Absolute and quadratic volumes of an element, of a mesh

Definition 9. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , the **absolute volume** volume $_t^{abs}(\mathcal{T}, \mathcal{V}_t)$ of an element $\mathcal{T} \in \mathcal{M}$ of vertices $P_{1,2,3}$ is the product of the area of \mathcal{T} by one third the sum of the absolute values of its three vertices:

volume
$$_t^{\text{abs}}(\mathcal{T}, \mathcal{V}_t) = \frac{\text{area}(\mathcal{T})}{3} \sum_{k=1}^{3} |\mathcal{V}_t(P_i)|$$
.

Definition 10. The absolute volume volume $_t^{abs}(\mathcal{M}, \mathcal{V}_t)$ of a mesh \mathcal{M} valuated at \mathcal{V}_t is the sum of the absolute volumes of its elements:

$$\operatorname{volume}_{t}^{\operatorname{abs}}(\mathcal{M},\,\mathcal{V}_{t}) = \sum_{\mathcal{T} \in \mathcal{M}} \operatorname{volume}_{t}^{\operatorname{abs}}(\mathcal{T},\,\mathcal{V}_{t}).$$

Proposition 2. The absolute volume of a mesh \mathcal{M} valuated at \mathcal{V}_t defined in definition 10 is invariant under sub-triangulation.

Proof. Analogous to the proof of proposition 1.

Definition 11. Given a mesh \mathcal{M} valuated at \mathcal{V}_t , the quadratic volume volume $_t^{\text{quad}}(\mathcal{T}, \mathcal{V}_t)$ of an element $\mathcal{T} \in \mathcal{M}$ is equal to the volume of \mathcal{T} valuated at \mathcal{V}_t^2 :

$$\operatorname{volume}_{t}^{\operatorname{quad}}(\mathcal{T}, \mathcal{V}_{t}) = \operatorname{volume}_{t}(\mathcal{T}, \mathcal{V}_{t}^{2}) = \frac{\operatorname{area}(\mathcal{T})}{3} \sum_{k=1}^{3} \mathcal{V}_{t}^{2}(P_{i}).$$

Definition 12. The quadratic volume volume $_t^{abs}(\mathcal{M}, \mathcal{V}_t)$ of a mesh \mathcal{M} valuated at \mathcal{V}_t is the square root of the sum of the quadratic volumes of its elements:

$$\operatorname{volume}_{t}^{\operatorname{quad}}(\mathcal{M},\,\mathcal{V}_{t}) = \sqrt{\sum_{\mathcal{T} \in \mathcal{M}} \operatorname{volume}_{t}^{\operatorname{quad}}(\mathcal{T},\,\mathcal{V}_{t})}.$$

Proposition 3. The quadratic volume of a mesh \mathcal{M} valuated at \mathcal{V}_t defined in definition 12 is invariant under sub-triangulation.

Proof. By definition,

$$volume_{t}^{quad}(\mathcal{M}, \mathcal{V}_{t}) = \sqrt{\sum_{\mathcal{T} \in \mathcal{M}} volume_{t}^{quad}(\mathcal{T}, \mathcal{V}_{t})}$$
$$= \sqrt{\sum_{\mathcal{T} \in \mathcal{M}} volume_{t}(\mathcal{T}, \mathcal{V}_{t}^{2})}$$
$$= \sqrt{volume_{t}(\mathcal{M}, \mathcal{V}_{t}^{2})},$$

yet by proposition 1, the volume of \mathcal{M} valuated at \mathcal{V}_t^2 is invariant under sub-triangulation, thus the quadratic volume of \mathcal{M} valuated at \mathcal{V}_t is also invariant under sub-triangulation.

6 Comparison between two meshes

6.1 Comparison between two identical meshes

Definition 13. Two meshes \mathcal{M}_1 and \mathcal{M}_2 are identical if the sets of their elements are equal:

$$\{\mathcal{T} \in \mathcal{M}_1\} = \{\mathcal{T} \in \mathcal{M}_2\}$$

.

Definition 14. A reference mesh is a mesh \mathcal{M}_0 with a constant valuation $\mathcal{V}_t = \mathcal{V}_0$ for all time t.

6.1.1 Mean signed deviation

Definition 15. Let \mathcal{M}_0 be a reference mesh with valuation \mathcal{V}_0 . For any mesh valuated at \mathcal{V}_t and identical to \mathcal{M}_0 , the **mean signed deviation (MSD)** with respect to \mathcal{M}_0 is the function $MSD_{\mathcal{M}_0,\mathcal{V}_0}$ in \mathbb{R}_+ that maps $(\mathcal{M}_0,\mathcal{V}_t)$ to the volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$, divided by the total area of \mathcal{M}_0 :

$$\mathrm{MSD}_{\mathcal{M}_0,\mathcal{V}_0}(\mathcal{M}_0,\,\mathcal{V}_t) = \frac{\mathrm{volume}_t(\mathcal{M}_0,\mathcal{V}_t - \mathcal{V}_0)}{\mathrm{area}(\mathcal{M}_0)}.$$

Proposition 4. The mean signed distance is invariant under sub-triangulation.

Proof. It is clear that a sub-triangulation does not change the total area of the mesh. By proposition 1, the volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$ is invariant under sub-triangulation. Therefore the mean signed deviation is also invariant under sub-triangulation.

6.1.2 Mean absolute deviation

Definition 16. Let \mathcal{M}_0 be a reference mesh with valuation \mathcal{V}_0 . For any mesh valuated at \mathcal{V}_t and identical to \mathcal{M}_0 , the **mean absolute error (MAD)** with respect to \mathcal{M}_0 is the function $\text{MAD}_{\mathcal{M}_0,\mathcal{V}_0}$ in \mathbb{R}_+ that maps $(\mathcal{M}_0, \mathcal{V}_t)$ to the absolute volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$, divided by the total area of \mathcal{M}_0 :

$$MAD_{\mathcal{M}_0, \mathcal{V}_0}(\mathcal{M}_0, \mathcal{V}_t) = \frac{\text{volume}_t^{\text{abs}}(\mathcal{M}_0, \mathcal{V}_t - \mathcal{V}_0)}{\text{area}(\mathcal{M}_0)}.$$

Proposition 5. The mean absolute distance is invariant under sub-triangulation.

Proof. It is clear that a sub-triangulation does not change the total area of the mesh. By proposition 2, the absolute volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$ is invariant under sub-triangulation. Therefore the mean absolute deviation is also invariant under sub-triangulation.

6.1.3 Root mean square deviation

Definition 17. Let \mathcal{M}_0 be a reference mesh with valuation \mathcal{V}_0 . For any mesh valuated at \mathcal{V}_t and identical to \mathcal{M}_0 , the **root mean square deviation (RMSD)** with respect to \mathcal{M}_0 is the function RMSD $_{\mathcal{M}_0,\mathcal{V}_0}$ in \mathbb{R}_+ that maps $(\mathcal{M}_0,\mathcal{V}_t)$ to the quadratic volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$, divided by the total area of \mathcal{M}_0 :

$$\mathrm{RMSD}_{\mathcal{M}_0,\mathcal{V}_0}(\mathcal{M}_0,\,\mathcal{V}_t) = \frac{\mathrm{volume}_t^{\mathrm{quad}}(\mathcal{M}_0,\mathcal{V}_t - \mathcal{V}_0)}{\mathrm{area}(\mathcal{M}_0)}.$$

Proposition 6. The root mean square deviation is invariant under sub-triangulation.

Proof. It is clear that a sub-triangulation does not change the total area of the mesh. By proposition 3, the quadratic volume of \mathcal{M}_0 valuated at $\mathcal{V}_t - \mathcal{V}_0$ is invariant under sub-triangulation. Therefore the root mean square deviation is also invariant under sub-triangulation.

6.1.4 Element-wise signed deviation, deviation distribution

Let \mathcal{M}_0 be a reference mesh with valuation \mathcal{V}_0 . For any mesh valuated at \mathcal{V}_t and identical to \mathcal{M}_0 , the **deviation distribution function** F_X is the empirical distribution function of the variable

$$X = \frac{\operatorname{size}(\mathcal{M}_0) \operatorname{volume}_t(\mathcal{T}, \mathcal{V}_t - \mathcal{V}_0)}{\operatorname{area}(\mathcal{M}_0)},$$

called the **element-wise signed deviation**, measured from the set of all elements $\mathcal{T} \in \mathcal{M}_0$:

$$F_X(x) = \frac{1}{\operatorname{size}(\mathcal{M})}\operatorname{card}\left\{\mathcal{T} \in \mathcal{M}_0 \mid \frac{\operatorname{size}(\mathcal{M})\operatorname{volume}_t(\mathcal{T}, \mathcal{V}_t - \mathcal{V}_0)}{\operatorname{area}(\mathcal{M})} \leqslant x\right\}, \quad x \in \mathbb{R}.$$

Remark 1. The empirical mean of the element-wise signed deviation is equal to the mean signed deviation defined in 15:

$$\mathbb{E}(X) = \frac{1}{\operatorname{size}(\mathcal{M}_0)} \sum_{\mathcal{T} \in \mathcal{M}_0} \left(\frac{\operatorname{size}(\mathcal{M}_0) \operatorname{volume}_t(\mathcal{T}, \mathcal{V}_t - \mathcal{V}_0)}{\operatorname{area}(\mathcal{M}_0)} \right)$$

$$= \sum_{\mathcal{T} \in \mathcal{M}_0} \left(\frac{\operatorname{volume}_t(\mathcal{T}, \mathcal{V}_t - \mathcal{V}_0)}{\operatorname{area}(\mathcal{M}_0)} \right)$$

$$= \frac{\operatorname{volume}_t(\mathcal{M}_0, \mathcal{V}_t - \mathcal{V}_0)}{\operatorname{area}(\mathcal{M}_0)}$$

$$= \operatorname{MSD}_{\mathcal{M}_0, \mathcal{V}_0}(\mathcal{M}_0, \mathcal{V}_t),$$

and is therefore invariant under sub-triangulation.