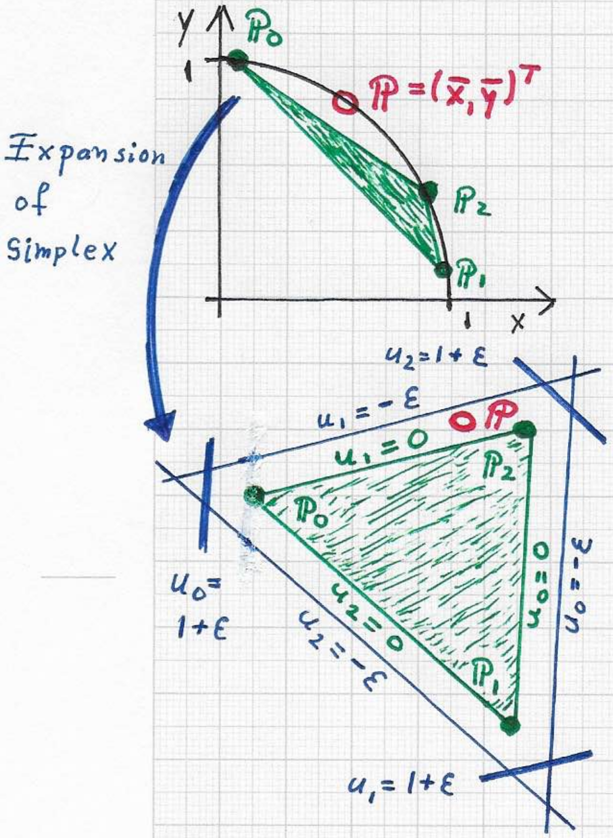
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: The figure (left, top) is merely provided again to remind us that the simplices we are concerned with have vertices $\mathbb{P}_0, \mathbb{P}_1, \mathbb{P}_2, \ldots$ that have NORMALIZED positional vectors. Thus, the point $\mathbb{P}$ lies OUTSIDE the (shaded) region implied by $\mathbb{P}_0, \mathbb{P}_1, \mathbb{P}_2, \ldots$, i.e., the CONVEX simplex region. The point $\mathbb{P}$ can, of course, still be written as $\mathbb{P} = \sum_{i=0}^{k-1} u_i \mathbb{P}_i$, but the u_i-values only satisfy the "partition of unity" property, i.e., $\sum_{i=0}^{k-1} u_i = 1$; they cannot and do not satisfy the "non-negativity" property, i.e., $u_i \geq 0,\ i=0,\ldots,k-1$. The figure (left, bottom) shows that one expand a simplex region via the use of barycentric coordinate values that describe an "ε-strip"/"ε-band" around the "exact" simplex region by using intervals:

$$u_i \in [-\varepsilon, 1+\varepsilon]\ , i=0,\ldots,k$$

This concept is important to keep in mind, since the point $\mathbb{P}$ has coordinate values "slightly" below 0 or above 1 and still can represent a (sample) class $\mathbb{P}_i$. ...



Illustrations of the "exact" 2-simplex and point $\mathbb{P}$ to be represented as a barycentric combination, with an added ε-band in the bottom figure.

In the specific example (bottom), the point $\mathbb{P}$ has coordinate values

$$0 < u_0 < 1\ ,\quad -\varepsilon < u_1 < 0\ ,\quad 0 < u_2 < 1\ ,$$

but it should still be viewed as being of (sample) class $\mathbb{P}_1$ – since the point $\mathbb{P}$ is inside the ε-strip.

▪ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: … The points p_i, i.e., the simplex vertices, can be thought of as single samples of a specific (material) class or as multiple "allowable and possible" samples of just one (material) class. Regardless of the view taken, the basic question concerning a new unclassified point p is the same in both scenarios: "Is p close enough to any of the points p_i so that it is possible to view p as yet another instance/representative of p_i, potentially involving an associated probability based on the distance between p and p_i?" We have introduced a point's barycentric coordinate tuple, relative to a reference simplex, as a means to determine a measure for similarity between the point and the simplex vertices. This approach is closely related to a problem arising in computational material science: material interface (re-)construction from so-called "volume fraction simulations." (See: Kathleen Bonnell et al., "Material Interface Reconstruction," IEEE Trans. Visualization and Comp. Graphics, 2003.)

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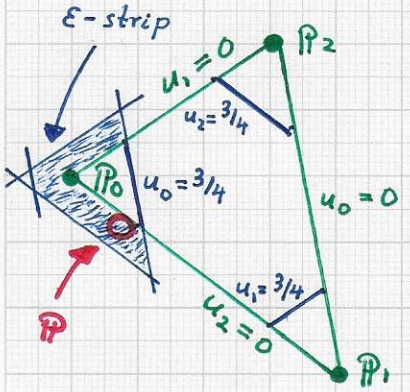


Simplistic method and condition for recognizing point p as yet "another instance of class p_0": The barycentric coordinates of p satisfy

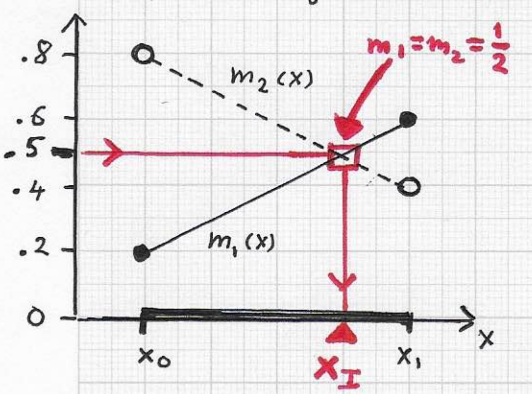
$$3/4 \le u_0 \le 1+\varepsilon,$$
$$-\varepsilon \le u_1 (\le \dots),$$
$$-\varepsilon \le u_2 (\le \dots).$$

The specific value $3/4$ is merely exemplary; this value, together with the value of ε, would have to be determined via an optimization and "training" process with application-specific data.

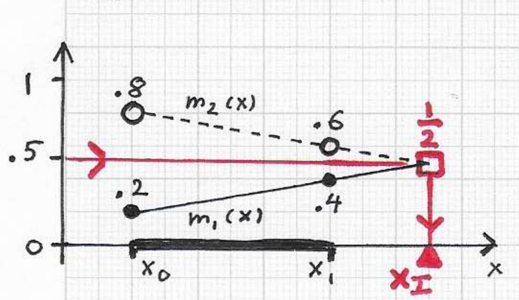
The points/vertices p_i, $i=0,1,2$, have barycentric coordinate tuples $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$. These tuples can be viewed as **VOLUME FRACTION** tuples – with only one material present at a vertex p_i.

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... We are concerned with answering a classification question: "Given a simplex with uniquely classified vertices p_i and the unclassified point p, can p be viewed as another representative of point class p_i or not?" In the context of material interface construction, the question one wants to answer is different, it is: "Given a simplex with vertex-associated material volume fraction tuples, defining the fraction of one of several material 'present' at each vertex, where are the GEOMETRICAL interfaces between different-material regions inside the simplex?" One can consider the material interface construction method in the context of material classification. We briefly describe the essential idea of interface definition and calculation by using a **2-material example** for a one-dimensional (x-axis) domain, see figures (left).



Determining the location of the interface between material m_1 and m_2 data. The given data consists of the locations x_0 and x_1 with associated fractional material tuples (.2, .8) and (.6, .4), respectively. The interface location in the x-domain is defined as the location where $m_1(x) = m_2(x) = .5$. The functions $m_1(x)$ and $m_2(x)$ are the two linear functions that interpolate the given data at x_0 and x_1.



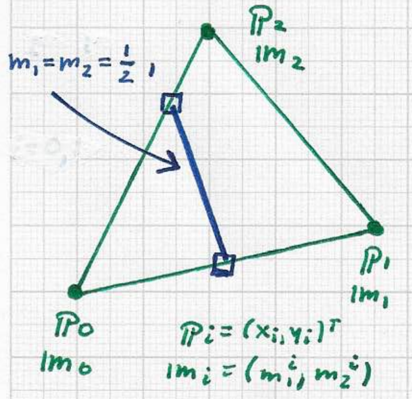
The top example shows a case where the interface location x_I lies inside the interval $[x_0, x_1]$, while the bottom example leads to a location outside this interval.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacion eigenfunctions: ... In the 2-material case shown, we have two 2-material tuples $\mathbb{m}_0 = (m_1^0, m_2^0)$ and $\mathbb{m}_1 = (m_1^1, m_2^1)$ associated with x-axis locations x_0 and x_1, respectively. One can use linear interpolation to blend the tuples $\mathbb{m}_0$ and $\mathbb{m}_1$, i.e.,

$$\mathbb{m}(x) = \frac{x_1 - x}{x_1 - x_0}\,\mathbb{m}_0 + \frac{x - x_0}{x_1 - x_0}\,\mathbb{m}_1 .$$



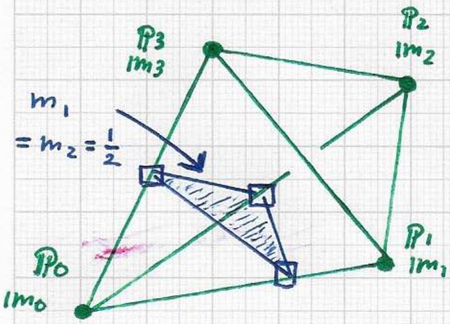
Material interface of 2 materials constructed for a 2-simplex. Ignoring singular and degenerate cases, a 2-simplex can only be "split" in this way when an interface exists in its interior.

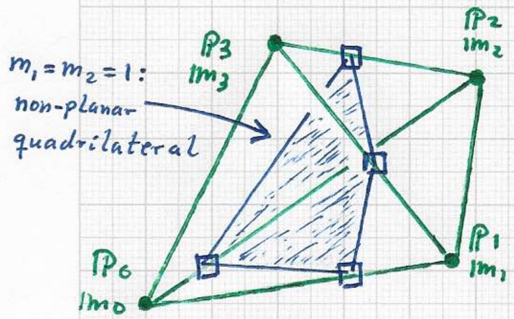
Thus, the individual material component functions are

$$m_i(x) = \frac{x_1 - x}{x_1 - x_0}\, m_i^0 + \frac{x - x_0}{x_1 - x_0}\, m_i^1 \, , \; i = 1, 2.$$

The "interface location" x_I is defined by the condition $m_1(x_I) = m_2(x_I) = \frac{1}{2}$.

One obtain the value of x_I by solving $m_i(x) = \ldots = \frac{1}{2}$ for x. (A special case arises when the material component functions are constant functions.) In other words, the "interface location" is the location where the **dominance** of one material over the other changes.





Material interfaces of 2 materials for a 3-simplex. A triangle or non-planar quadrilateral can result.

• **Note.** Via re-parametrization to the t-line and the interval $0 \le t \le 1$, one can write the linearly interpolating function as $m(t) = (1-t)m_0 + t m_1$, which has the value 1/2 for $t_I = \frac{1 - 2m_0}{2(m_1 - m_0)}$. Thus, one obtains the value for x_I: $x_I = (1 - t_I)x_0 + t_I x_1$.

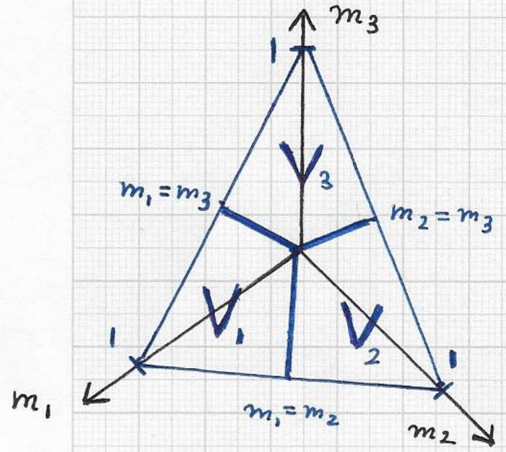
...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

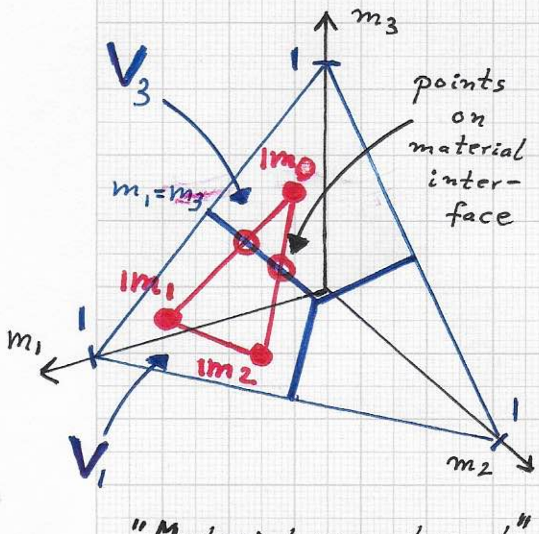
• Laplacian eigenfunctions: ... We briefly summarize the relationship between "material space" to describe fractional material tuples $(m_1, m_2, \ldots)$ and "physical space" to describe the geometry of a simplex with vertices $\mathbb{p}_0, \mathbb{p}_1, \ldots$ We consider the case of three material classes, i.e., tuples (m_1, m_2, m_3), that are associated as fractional data with the vertices of a 2-simplex. The given data are tuples $\mathbb{m}_i = (m_1^i, m_2^i, m_3^i)$ that are attached to vertices $\mathbb{p}_i = (x_i, y_i)^T$, $i = 0, 1, 2$. Since the fractional material tuples represent physical area (or volume) fractions, they must satisfy the conditions

$$\sum_{j=1}^{3} m_j = 1 \;\wedge\; m_j \geq 0 .$$

The figure (left, top) shows the allowable region (= triangle) of $\mathbb{m}$-tuples. Using the idea of a Voronoi tessellation, one can 'naturally' split the allowable region into Voronoi tiles V_j. An $\mathbb{m}$-tuple can lie inside any tile, and one can 'postulate' the existence of a material interface along a line segment $\overline{\mathbb{m}_1 \mathbb{m}_2}$ when the endpoints lie in different tiles. (See left figure, bottom.) ...



Material space for 3 materials m_1, m_2 and m_3. The finite convex region satisfying $m_1 + m_2 + m_3 = 1$ and $m_j \geq 0$ can be tessellated via 3 Voronoi tiles V_j.



"Material space triangle" with corner tuples $\mathbb{m}_i$, $i = 0, 1, 2$, contains an interface between materials m_1 and m_3, as segments $\overline{\mathbb{m}_0 \mathbb{m}_1}$ and $\overline{\mathbb{m}_0 \mathbb{m}_2}$ intersect with $m_1 = m_3$.