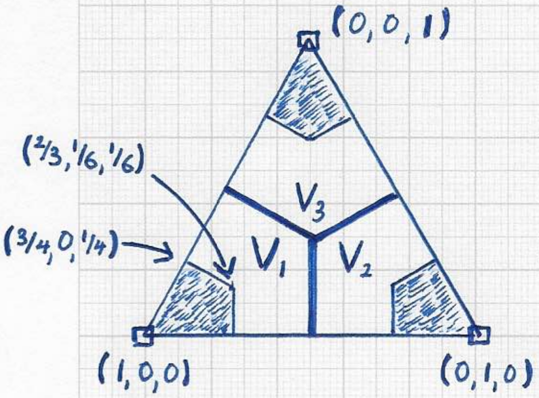
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: … For our driving data classification problem, the number of material classes must be assumed to be "relatively large." An explicit complex computation of the "postulated" material interfaces – and their representation with complex and storage-intensive data structures – is not feasible. **It must also be noted that designating locations in "material space" where material volume fractions are equal ($m_i = m_j$) as material interfaces is (practically) NOT the proper approach for determining the "best" boundaries of regions defining the allowable m-domains for specific material classes.** The reviewed material interface (re-) construction method computes a (clipped) Voronoi tessalation with a set of tiles V_i that – together – represent the entire region that satisfies $m_1 + \ldots + m_K = 1$ and $m_i \geq 0$. **But: In practice, one must assume that many m-tuples in this region do NOT belong to a specific class.** …



Original Voronoi tiles V_1, V_2 and V_3 for three-material case and "scaled-down" tiles (shaded). "Down-scaling" of tiles should generate "material space" regions that optimally cover the space of allowable m-tuples representing material classes 1, 2 and 3.

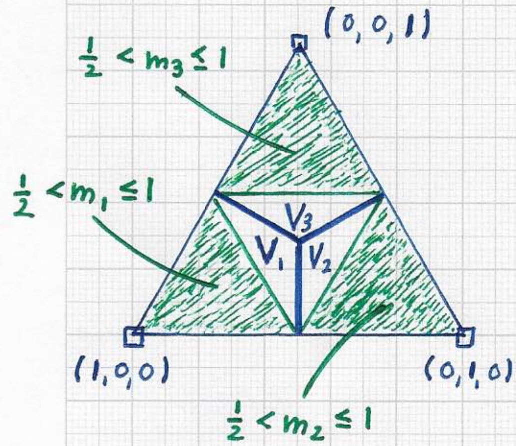
The original tile V_1 – the "tile of material-1 tuples" – contains a large sub-region where m-tuples should NOT be classified as material-1 tuples. For example, m-tuples (m_1, m_2, m_3) for which

$$m_1 < (m_2 + m_3)$$

holds should most likely not be classified as tuples of material class 1.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... Therefore, while the geometrical definition and structure of the "material space" Voronoi tesselation is elegant, one must much more carefully determine tiles V_i that "correctly" describe the region containing "ALL AND ONLY" the allowable $\mathbb{m}$-tuples of material class i. For example, one could consider a solution approach to this problem by scaling down the Voronoi tiles of the initial Voronoi tessellation. For the purpose of practical data classification, it would be crucial to perform the "best possible" scaling of a tile to ensure that an $\mathbb{m}$-tuple is only classified as a tuple of material class i when it should be. Thus, "proper and sufficient" training with actual samples is essential. Instead of geometrically scaling down the Voronoi tiles, as shown in the figure on the previous page, one can also require that $\frac{1}{2} < m_i \leq 1$ to define a sub-region in Voronoi tile V_i, see figure (left). ...



Original Voronoi tiles V_1, V_2 and V_3 for three-material case and tile sub-regions where the values of m_1, m_2 and m_3, respectively, are above 1/2 and smaller than or equal to 1.

The sub-region of Voronoi tile V_1 where the value of m_1 satisfies

$$\frac{1}{2} < m_1 \leq 1$$

contains only $\mathbb{m}$-tuples where material 1 is "dominant" in the sense that the sum of all other material values is not larger than the value of m_1, i.e.,

$$m_1 > (m_2 + m_3).$$

Even though the material 1 is the "dominant" material per m_1-value, it might still be incorrect to classify it as material 1.

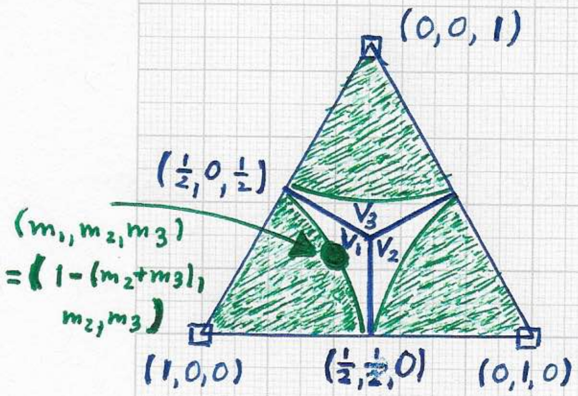
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... There exists yet another "natural way" one can consider to define a sub-region in Voronoi tile V_i to be considered the region associated with an m-tuple representing material class i, see figure (left). Considering Voronoi tile V_1, for example, the "Euclidean distance" between m-tuples $(1,0,0)$ and $(\frac{1}{2},\frac{1}{2},0)$ is $\left((1-\frac{1}{2})^2+(-\frac{1}{2})^2+0^2\right)^{1/2}$. This value – $d_{max}=\sqrt{2}/2$ – can be used to establish the radius of a cirle / circular arc with center $(1,0,0)$, bounding the shaded sub-region in the figure. The figure shows an m-tuple (m_1,m_2,m_3) on the bounding circular arc. The distance d of this m-tuple and $(1,0,0)$ is

$$d = \left((m_2+m_3)^2+(-m_2)^2+(-m_3)^2\right)^{1/2}$$
$$= \left(m_2^2+2m_2m_3+m_3^2+m_2^2+m_3^2\right)^{1/2}$$
$$= \left(2m_2^2+2m_2m_3+2m_3^2\right)^{1/2}$$
$$= \sqrt{2}\left(m_2^2+m_2m_3+m_3^2\right)^{1/2}$$

An m-tuple $m=(m_1,m_2,m_3)=(1-(m_2+m_3),m_2,m_3)$ lying on the bounding circular arc and satisfies the condition $d=d_{max}=\sqrt{2}/2$.

Thus, $\left(m_2^2+m_2m_3+m_3^2\right)^{1/2}=\frac{1}{2}$. ...



Original Voronoi tiles V_1, V_2 and V_3 for three-material case and tile sub-regions defined by requirement that the "Euclidean distance" between an m-tuple and the "corner point" □ of a tile is smaller than $d=\sqrt{2}/2=d_{max}$.

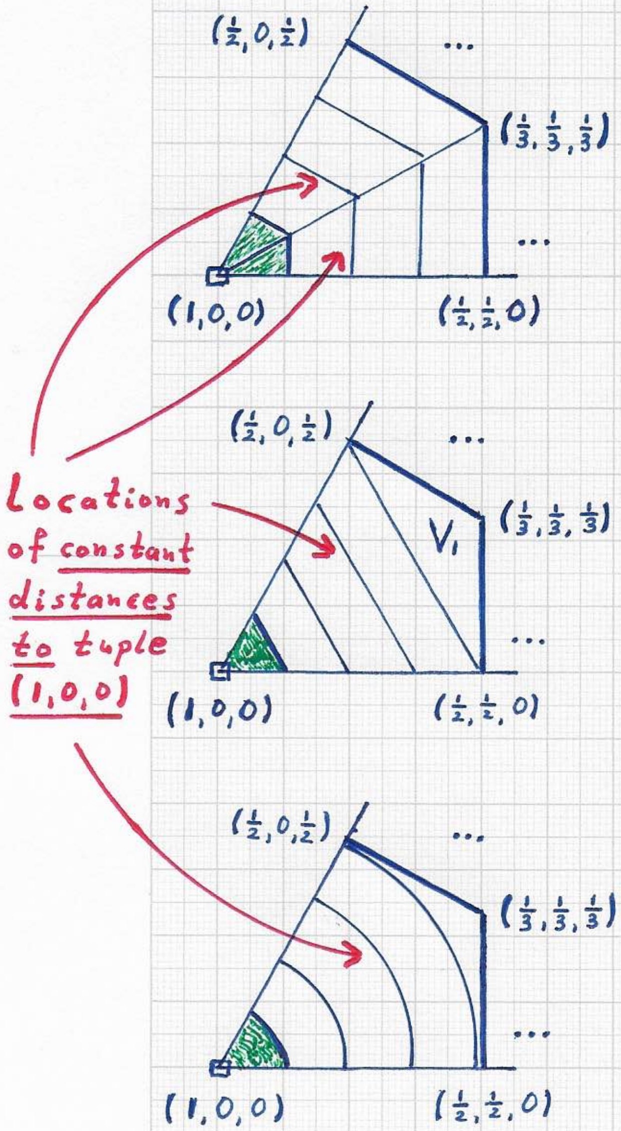
The sub-region of Voronoi tile V_1 where the length of the difference vector $(m_1,m_2,m_3)-(1,0,0)$ is smaller than a maximal radius d_{max} can be used to define the region of m-tuples viewed as material-1 tuples.

Thus, the length is

$$\|(1,0,0)-(1-(m_2+m_3),m_2,m_3)\|.$$

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... The geometrical principles of scaling-down an original Voronoi tile are summarized for the simple three approaches considered. The goal is to define a sub-region in the Voronoi tile V_i that covers – in the "best possible way" – the region of m-tuple values that truly belong to material class 1 (in the specific example shown in the figures). The first approach scales Voronoi tile V_1, making it smaller and preserving its native shape (top figure). The second approach uses lines (hyper-planes) of constant m_1-values to define the part of a sub-region's boundary that is inside the original simplex (middle figure). The third approach establishes disks, centered at "pure" materials' m-tuples, as sub-regions in tiles V_i, with a circular arc (part of a hyper-sphere) being the boundary in the Voronoi tiles' interior (bottom figure). The three kinds of "isolines"/"isocurves" shown in the three figures can also be understood as locations where the values of some "DISTANCE TO (1,0,0)" are constant. ...



Three simple possibilities to shrink / scale-down the original Voronoi tile V_1 associated with the "pure" m-tuple (1,0,0).
Top: Sub-region is a scaled-down "copy" of tile V_1.
Middle: Sub-region is a scaled-down "copy" of the original 2-simplex.
Bottom: Sub-region is a (part of) a disk with center (1,0,0).

▪ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... The figures (left) illustrate the three distance measures. The top figure shows isolines of the simplest distance to the "pure" $\mathbb{m}$-tuple $(1,0,0)$:

$$d = 1 - m_1 \quad , \quad 0 \le m_1 \le 1 \ .$$

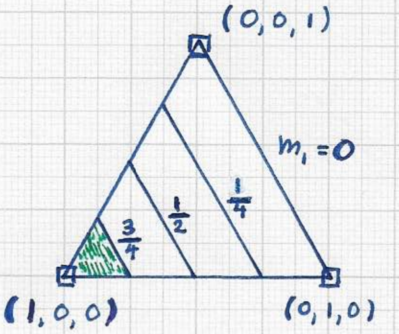
Thus, d also varies between 0 and 1, considering the entire simplex. By requiring that $0 \le m_1 \le \frac{1}{2}$ one ensures that $\mathbb{m}$-tuples satisfying this requirement lie inside Voronoi tile V_1. The middle figure (left) shows how one can employ a circular arc (a part of a hyper-sphere in general) to bound a sub-region (with hyper-sphere center $(1,0,0)$). The distance between $(1,0,0)$ and $\mathbb{m} = (m_1, m_2, m_3) = (1-(m_2+m_3), m_2, m_3)$ is

$$\begin{aligned} d &= \left((m_2+m_3)^2 + m_2^2 + m_3^2 \right)^{1/2} \\ &= \left(2m_2^2 + 2m_2m_3 + 2m_3^2 \right)^{1/2} \\ &= \sqrt{2} \left(m_2^2 + m_2m_3 + m_3^2 \right)^{1/2} , \end{aligned}$$

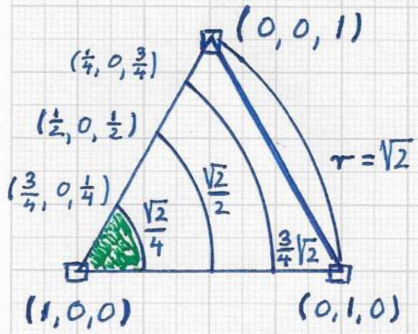
$$0 \le m_2, m_3 \le 1 \wedge m_2 + m_3 \le 1 .$$

Considering $\mathbb{m}$-tuples $(m_1, 0, m_3)$ on the simplex edge connecting $(1,0,0)$ and $(0,0,1)$, one obtains $d = \sqrt{2} \cdot m_3$. Thus, the radii r of the five concentric circular arcs in the figure (left, bottom) are $0, \sqrt{2}/4, \sqrt{2}/2, 3\sqrt{2}/4, \sqrt{2}$.

...



Simplest way of defining the sub-region boundary inside the simplex: $0 \le m_1 \le 1$.



Defining the sub-region boundary inside the simplex via radius of hyper-sphere.

A sub-region inside the simplex is bounded in the interior of the simplex by a circular arc (2-simplex case).

By requiring that $0 \le m_2, m_3 \le 1/2 \wedge m_2 + m_3 \le 1/2$ one ensures that $\mathbb{m}$-tuples satisfying this requirement lie inside Voronoi tile V_1.