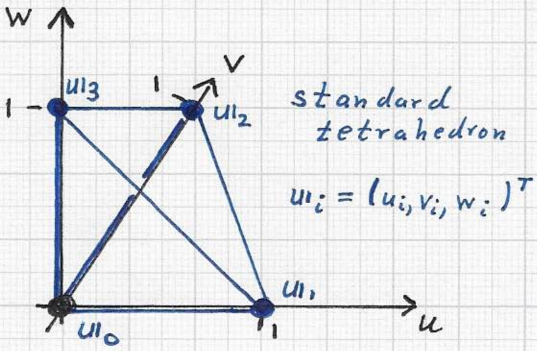
Bernd Hamann

Stratovan

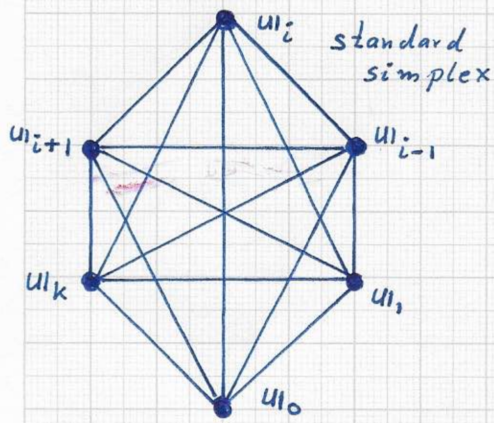
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ...



Compute volume of standard tetrahedron via trivariate integration:

$$\text{volume}(\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3) = \int_{u=0}^{1} \int_{v=0}^{1-u} \int_{w=0}^{1-u-v} 1 \, dw\, dv\, du = \ldots = \frac{1}{6}$$



k+1 simplex vertices

$$\begin{bmatrix} \mathbf{u}_0 = (0, 0, \ldots, 0, 0)^T \\ \mathbf{u}_1 = (1, 0, \ldots, 0, 0)^T \\ \mathbf{u}_{k-1} = (0, 0, \ldots, 1, 0)^T \\ \mathbf{u}_k = (\underbrace{0, 0, \ldots, 0, 1}_{k \text{ coordinates}})^T \end{bmatrix}$$

"Projection" of standard **k**-simplex with **k+1** vertices.

The figure (left, top) shows the standard tetrahedron in three-dimensional uvw-space. Its volume is calculated via trivariate, triple integration; the volume is $\text{volume}(\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3) = \frac{1}{3!} = \frac{1}{6}$. The volume of the standard simplex in **k**-dimensional space, shown as a graph, a "projection" (left figure, bottom), can be derived via induction or direct multi-variate integration. The volume is given as

$$\text{volume}(\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k) = \int_{u_1=0}^{1} \int_{u_2=0}^{1-u_1} \int_{u_3=0}^{1-u_1-u_2} \cdots \int_{u_k=0}^{1-u_1-u_2-\ldots-u_{k-1}} 1 \; du_k \ldots du_1 = \frac{1}{k!} \, .$$

!

The linear mapping that maps the points $\mathbf{u}_i$, $i = 0, \ldots, k$, to corresponding points $\mathbf{x}_i$, $i = 0, \ldots, k$ – i.e., $\mathbf{u}_i \mapsto \mathbf{x}_i$ – is written as $\mathbf{x}(\mathbf{u}) = A\mathbf{u} + \mathbf{b}$.

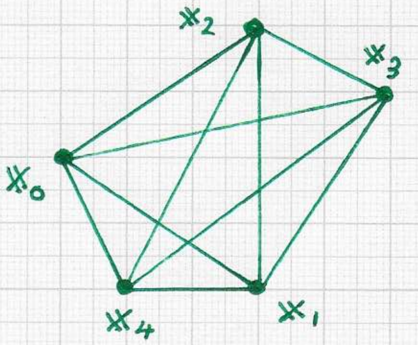
The images of the unit/normalized basis vectors $\mathbf{u}_i - \mathbf{u}_0$, $i = 1, \ldots, k$, are the vectors $\mathbf{x}_i - \mathbf{x}_0$, $i = 1, \ldots, k$.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

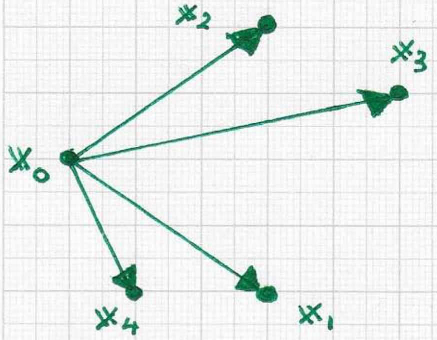
• Laplacian eigenfunctions: ... The columns of the matrix A are the image vectors $\mathbf{x}_i - \mathbf{x}_0$, $i = 1, \dots, k$. Therefore, the Jacobian J is

$$J = \left| \begin{array}{c|c|c} \mathbf{x}_1 - \mathbf{x}_0 & \dots & \mathbf{x}_k - \mathbf{x}_0 \end{array} \right| .$$



Example (k=4) of a simplex projected from four-dimensional space with vertices $\mathbf{p}_i = \mathbf{x}_i$.

⇒ THE SIGNED VOLUME OF A SIMPLEX IN k-DIMENSIONAL SPACE IS $J/k!$ * **!**



Corresponding image vectors $\mathbf{x}_i - \mathbf{x}_0$, $i = 1, \dots, 4$, defining the Jacobian J.

Thus, the use of the change-of-variables theorem provides us with another means of the computation of signed simplex volumes of k-simplices in k-dimensional space with (k+1) vertices. Again, we want to express a given point $\mathbf{p}$ in k-dimensional space relative to a "reference k-simplex." This representation of $\mathbf{p}$ requires us to compute $\mathbf{p}$'s barycentric coordinates, i.e., ratios of signed k-simplex volumes.

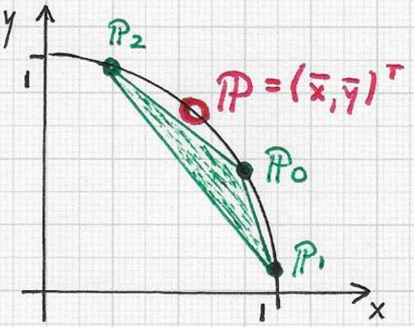
! • Cramer's rule for solving linear equation systems and the change-of-variables theorem used for simplex volume computations are equivalent ways to calculate barycentric coordinates.

* Given two simplices with volumes $J_1/k!$ and $J_2/k!$, their volume ratio is J_1/J_2. Thus, the factor $1/k!$ does not matter for barycentric coord. computation.

...

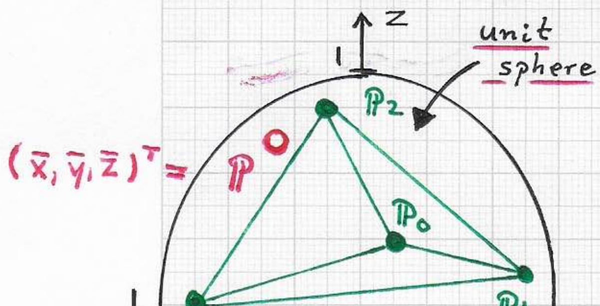
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... In summary, one can approach the computation of barycentric coordinates with different algorithmic methods. For a specific application setting one should employ the method that satisfies requirements regarding simplicity, numerical robustness and computational efficiency.



Example of a low-dimensional case: A 2-simplex/triangle in 2-dimensional space defined by 3 vertices $\mathbb{P}_0$, $\mathbb{P}_1$ and $\mathbb{P}_2$. The point $\mathbb{P}$ is represented relative to the "reference triangle" in barycentric coordinates. Since all the points involved represent NORMALIZED HISTOGRAM DATA, $\mathbb{P}$ always lies outside the triangle.

We can now consider the use of barycentric coordinates for object/material classification purposes: A material class is represented, described via a set of samples; the samples are characterized via distributions, histograms, of certain features, e.g., the distributions of coefficient values of multi-scale eigenfunction expansions. To determine whether a given not-yet-classified sample "matches in some probabalistic sense" one can compare histogram data of the given sample with histogram data of known material classes – USING BARYCENTRIC COORDINATES.

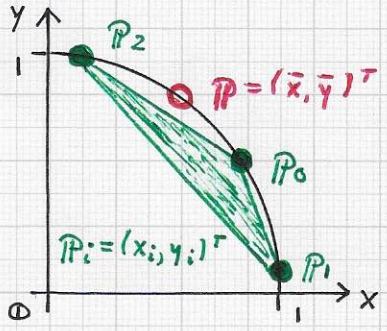


A 3-simplex/tetrahedron in 3-dimensional space defined by 4 vertices. The point $\mathbb{P}$ must be represented in barycentric coordinates.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions: ... One can consider slightly different classification scenarios: If one has **k** samples of the same material class available — "k sample histograms belonging to the same class" — then one will compare this data with the data of a not-yet-classified new sample; this scenario describes the case of determining whether a new sample is (is not) similar to a specific material class represented by k (classified) samples. If one has **k** samples (all classified) of **k** different materials available — "one sample histogram for each of the **k** classes" — then one will compare the data of a not-yet-classified sample with data representing **k** classes. Concerning both scenarios, the **k** classified sample data define **k** vertices of a (k-1)-simplex in (k-1)-dimensional space; the not-yet-classified new sample defines a point in (k-1)-dimensional space, and this point is represented in barycentric coordinates relative to the (k-1)-simplex. ...

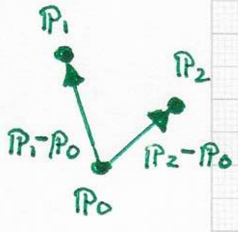


Classification scenario: The points $\mathbb{P}_i$ represent normalized histogram data of **3** samples, all classified. They define a **2-simplex**. The "unclassified point" $\mathbb{P}$ is represented in **2**-dimensional space relative to the **2**-simplex as $\mathbb{P} = u_0 \mathbb{P}_0 + u_1 \mathbb{P}_1 + u_2 \mathbb{P}_2$.

The barycentric coordinate values are

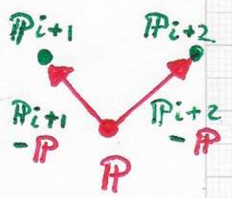
$$u_i = J_i / J \quad ,$$

where the Jacobian determinants J and J_i are



$$J = \begin{vmatrix} | & | \\ \mathbb{P}_1 - \mathbb{P}_0 & \mathbb{P}_2 - \mathbb{P}_0 \\ | & | \end{vmatrix}$$

and

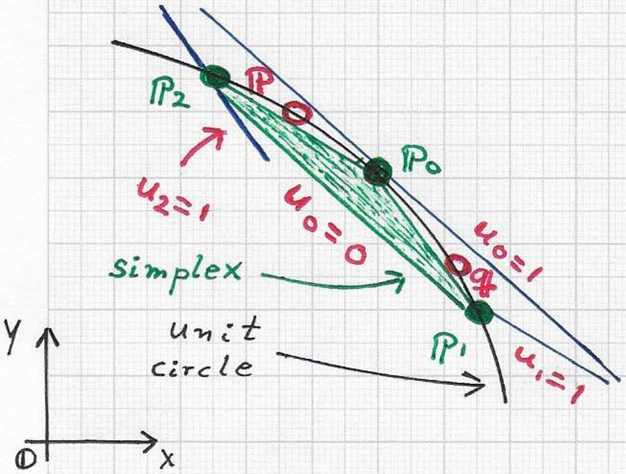


$$J_i = \begin{vmatrix} | & | \\ \mathbb{P}_{i+1} - \mathbb{P} & \mathbb{P}_{i+2} - \mathbb{P} \\ | & | \end{vmatrix} ,$$

$i = 0, 1, 2$, with all indices modulo **3**, i.e., using the index triples 012, 120 and 201.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ...



The point $\mathbb{P}$ to be represented via barycentric coordinates lies outside the "reference simplex/triangle. The point $\mathbb{q}$ is outside as well.

Considering the specific locations of $\mathbb{P}$ and $\mathbb{q}$ in this figure, the values of their barycentric coordinates lie in these ranges:

$\mathbb{P}$: $0 < u_0 < 1$, $-1 < u_1 < 0$, $0 < u_2 < 1$

$\mathbb{q}$: $0 < u_0 < 1$, $0 < u_1 < 1$, $-1 < u_2 < 0$

In principle, the fact that a barycentric coordinate(s) of a "point to be classified" is negative (are negative) can be handled by the classification process.

One can use $\mathbb{P}$'s barycentric coordinates to determine whether $\mathbb{P}$ can be viewed as a point that represents a material class (material class sample) associated with $\mathbb{P}_i$ or not.

The geometry describing our specific problem and setting is illustrated in more detail in the figure (left). The "reference simplex has vertices $\mathbb{P}_0, \mathbb{P}_1$ and $\mathbb{P}_2$ that lie on a hyper-sphere of radius 1 with the origin 0 as its center. The volume bounded by the simplex is a convex region; thus, the point $\mathbb{P}$ – another point on the hyper-sphere – lies OUTSIDE the region bounded by the simplex. In mathematical terms, the point $\mathbb{P}$ is written as a barycentric combination $\mathbb{P} = \sum_{i=0}^{k-1} u_i \mathbb{P}_i$, where $\sum_{i=0}^{k-1} u_i = 1$ – and u_i-values can be positive or negative, thus permitting combinations that are **NOT** convex combinations (for which $u_i \geq 0$ would have to be satisfied). **For data analysis and classification purposes, one can now use the k-dimensional coordinate tuple $(u_0, u_1, \ldots, u_{k-1})$.** !

...