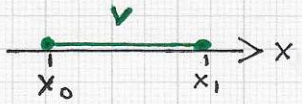
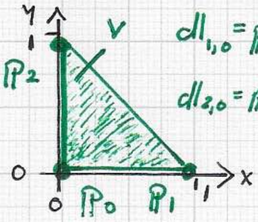
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

•Laplacian eigenfunctions: ...

Computation of (hyper-) volumes of simplices in arbitrary dimension



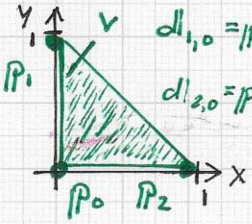
$$V = \frac{1}{1!} \det(x_1 - x_0) = \begin{cases} x_1 - x_0 \geq 0 & \text{if } x_1 \geq x_0 \\ x_1 - x_0 < 0 & \text{if } x_1 < x_0 \end{cases}$$



$dl_{1,0} = \mathbb{P}_1 - \mathbb{P}_0 = (1,0)^T$

$dl_{2,0} = \mathbb{P}_2 - \mathbb{P}_0 = (0,1)^T$

$$V = \frac{1}{2!} \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = \underline{\frac{1}{2}}$$

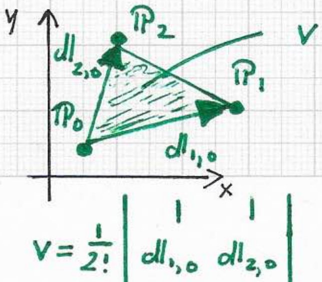


$dl_{1,0} = \mathbb{P}_1 - \mathbb{P}_0 = (0,1)^T$

$dl_{2,0} = \mathbb{P}_2 - \mathbb{P}_0 = (1,0)^T$

$$V = \frac{1}{2!} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} = \underline{-\frac{1}{2}}$$

Indexing/orientation defining sign of volume V of a simplex.



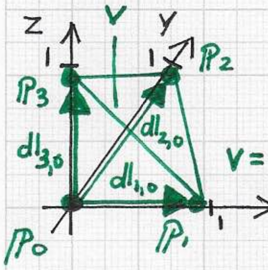
$$V = \frac{1}{2!} \begin{vmatrix} 1 & 1 \\ dl_{1,0} & dl_{2,0} \\ 1 & 1 \end{vmatrix}$$

HOW IS A SIMPLEX AND HOW ARE BARYCENTRIC COORDINATES RELATED TO THE CLASSIFICATION PROBLEM? We assume that a class is represented by k samples. Each sample is characterized statistically via a histogram, or multiple histograms, to describe a feature value's distribution. (In the case of an eigenfunction-based multi-scale/-frequency description of a sample, there are multiple, scale-specific coefficient value histograms – one histogram per scale.) **Each histogram has B = k bins.** (As discussed, one can construct a B-bin histogram such that B = k from an original histogram that has B ≠ k bins.) **After normalization, k histograms define k points on a unit hyper-sphere that is embedded in k-dimensional space. The "complete graph" of the k points defines a (k-1)-dimensional simplex – the "reference simplex."** ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

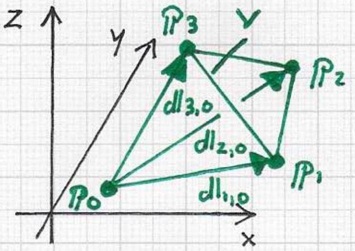
• Laplacian eigenfunctions:... WHEN A NEW UNCLASSIFIED SAMPLE IS GIVEN, IT IS ALSO CHARACTERIZED BY A NORMALIZED HISTOGRAM(S) DEFINING AN ADDITIONAL POINT(S) ON THE UNIT HYPER-SPHERE IN k-DIMENSIONAL SPACE. ONE CAN COMPUTE THE BARYCENTRIC COORDINATES OF THE NEW POINT(S) RELATIVE TO THE "REFERENCE SIMPLEX." THE RESULTING BARYCENTRIC COORDINATE VALUES FOR THE NEW POINT(S) ARE USED TO DETERMINE A PROBABILITY FOR THE NEW UNCLASSIFIED SAMPLE INDICATING WHETHER IT IS LIKELY FOR IT TO BELONG TO THE CLASS – EXEMPLIFIED BY THE k SAMPLES – OR NOT.

Simplex volumes:



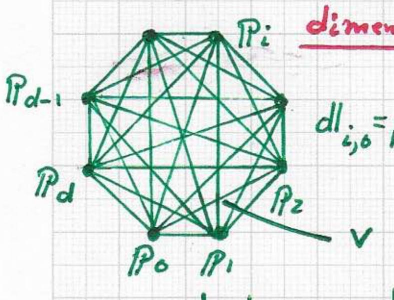
$dl_{i,0} = P_i - P_0$

$$V = \frac{1}{3!}\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{1}{6}$$



$$V = \frac{1}{3!}\begin{vmatrix} | & | & | \\ dl_{1,0} & dl_{2,0} & dl_{3,0} \\ | & | & | \end{vmatrix}$$

● General case:



dimension d

$dl_{i,0} = P_i - P_0$

$$V = \frac{1}{d!}\begin{vmatrix} | & & | \\ dl_{1,0} & \cdots & dl_{d,0} \\ | & & | \end{vmatrix}$$

Volumes of k-dimensional simplices in k-dimensional embedding space and (k+1) vertices.

The computation of signed hyper-volumes of simplices is necessary for the direct calculation of a point's barycentric coordinates. The previous, this and the following pages describe simplex volume computation.

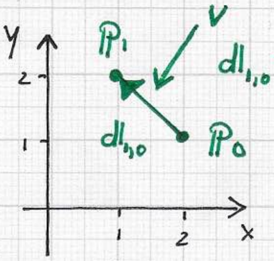
...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions: ... Considering the classification problem, the **k** "classified sample points" $\mathbb{P}_1, \ldots, \mathbb{P}_k$ are points with normalized positional vectors, i.e., they lie on a unit hyper-sphere of (manifold) dimension **(k-1)**, in a **k**-dimensional embedding space. Thus, one must compute volumes of **(k-1)**-dimensional simplices with vertices $\mathbb{P}_1, \ldots, \mathbb{P}_k$ in **k**-dimensional embedding space. The figures (left) show two examples, a 1- and 2-dimensional simplex (line segment and triangle), for which length and area are computed via square roots of determinants. **This volume computation can also be done via the calculation of the "cross product"* of vectors, i.e., via the calculation of normal vectors and their lengths.** The example (right figure) shows the computation of a line segment's absolute length value in 2-dimensional "embedding space."

Simplex volumes of (k-1)-dimensional simplices with k vertices, in k-dimensional embedding space:

k = 2



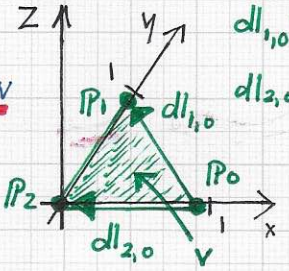
$$dl_{1,0} = \mathbb{P}_1 - \mathbb{P}_0 = (-1,1)^T$$

$$V = \frac{1}{1!}\left|\left(-dl_{1,0}-\right)\begin{pmatrix}|\\ dl_{1,0}\\ |\end{pmatrix}\right|^{1/2 \,*} = \left|(-1,1)\begin{pmatrix}-1\\ 1\end{pmatrix}\right|^{1/2} = \sqrt{2}$$

* The square root is taken of the absolute value of the determinant; THE SIGN OF THE DETERMINANT IS THE SIGN OF THE VOLUME.

!

k = 3



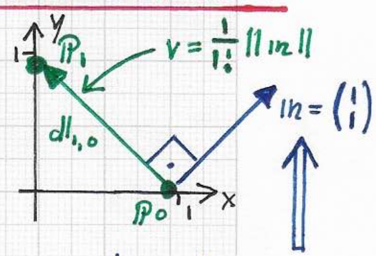
$$dl_{1,0} = (-1,1,0)^T \qquad dl_{2,0} = (-1,0,0)^T$$

$$V = \frac{1}{2!}\begin{vmatrix}\langle dl_{1,0}, dl_{1,0}\rangle & \langle dl_{1,0}, dl_{2,0}\rangle\\ \langle dl_{2,0}, dl_{1,0}\rangle & \langle dl_{2,0}, dl_{2,0}\rangle\end{vmatrix}^{1/2 \,*} = \frac{1}{2}\begin{vmatrix}2 & 1\\ 1 & 1\end{vmatrix}^{1/2} = \frac{1}{2}$$

• **General case: k**

$$V = \frac{1}{(k-1)!}\begin{vmatrix}\langle dl_{1,0}, dl_{1,0}\rangle & \ldots & \langle dl_{1,0}, dl_{k-1,0}\rangle\\ \vdots & & \vdots\\ \langle dl_{k-1,0}, dl_{1,0}\rangle & \ldots & \langle dl_{k-1,0}, dl_{k-1,0}\rangle\end{vmatrix}^{1/2 \,*}$$

* The "cross product" is defined only for some dimensions!



$$n: \begin{vmatrix}x & -1\\ y & 1\end{vmatrix} = \underline{\underline{1}}\,x + \underline{\underline{1}}\,y$$

$$\Rightarrow V = \|n\| = \sqrt{2}$$

...

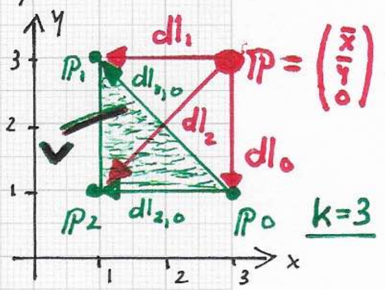
■ OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

• Laplacian eigenfunctions: ... **The normal's orientation defines the POSITIVE HALF-SPACE relative to the simplex: $+\mathbb{n}$ points in the positive half-space, and $-\mathbb{n}$ points in the negative half-space. The normal $+\mathbb{n}$ is also called "outward normal."** The indexing of the points $\mathbb{p}_0, \dots, \mathbb{p}_{k-1}$ defines the normal's orientation. As a consequence, a point's barycentric coordinates — **AND THEIR SIGNS** — depend on orientation. We provide a simple example of barycentric coordinate calculation (right figure). The "reference triangle" has vertices $\mathbb{p}_0, \mathbb{p}_1, \mathbb{p}_2$; its OUTWARD normal is defined by $\begin{vmatrix} x & -2 & -2 \\ y & 2 & 0 \\ z & 0 & 0 \end{vmatrix} = \underline{4} \cdot z \Rightarrow \mathbb{n} = (0,0,4)^T$. Thus, the volume of the triangle is $v = \frac{1}{2} \cdot 4 = 2$. The point $\mathbb{p}$ defines the 3 sub-triangles $\mathbb{p}\,\mathbb{p}_0\mathbb{p}_1$, $\mathbb{p}\,\mathbb{p}_1\mathbb{p}_2$ and $\mathbb{p}\,\mathbb{p}_2\mathbb{p}_0$ with their 3 normal vectors defined by

$$\begin{vmatrix} x & 0 & -2 \\ y & -2 & 0 \\ z & 0 & 0 \end{vmatrix}, \quad \begin{vmatrix} x & -2 & -2 \\ y & 0 & -2 \\ z & 0 & 0 \end{vmatrix} \text{ and } \begin{vmatrix} x & -2 & 0 \\ y & -2 & -2 \\ z & 0 & 0 \end{vmatrix}.$$

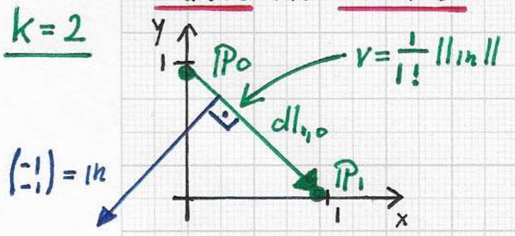
$$\mathrm{dl}_0 \ \mathrm{dl}_1 \qquad \mathrm{dl}_1 \ \mathrm{dl}_2 \qquad \mathrm{dl}_2 \ \mathrm{dl}_0$$

Thus, the normals of the sub-triangles are $\mathbb{n}_2 = (0,0,\underline{-4})^T$, $\mathbb{n}_0 = (0,0,4)^T$ and $\mathbb{n}_1 = (0,0,4)^T$. ...



(Hyper-) Volumes of Simplices — Determinants and normals:

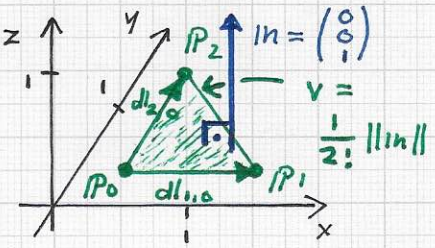
k=2



$\mathbb{n}: \begin{vmatrix} x & 1 \\ y & -1 \end{vmatrix} = \underline{-1}x \underline{-1}y$

$\Rightarrow v = \|\mathbb{n}\| = \sqrt{2}$

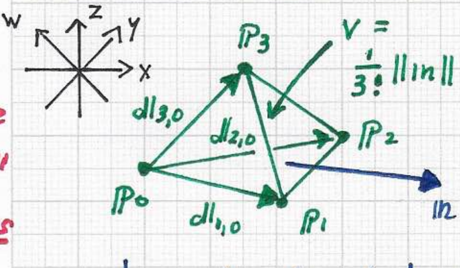
k=3



$\mathbb{n}: \begin{vmatrix} x & 1 & 0 \\ y & 0 & 1 \\ z & 0 & 0 \end{vmatrix} = \underline{0}\,x \underline{+0}\,y \underline{+1}\,z$

$\Rightarrow v = \frac{1}{2}\|\mathbb{n}\| = \frac{1}{2}$

k=4



$\mathbb{n}: \begin{vmatrix} x & | & | & | \\ y & \mathrm{dl}_{1,0} & \mathrm{dl}_{2,0} & \mathrm{dl}_{3,0} \\ z & & & \\ w & | & | & | \end{vmatrix} = \begin{matrix} Ax \\ +By \\ +Cz \\ +Dw \end{matrix}$

$\Rightarrow v = \frac{1}{6}\|(A,B,C,D)^T\|$

• **Note:** The "standard" vector cross product cannot be applied to arbitrary dimension!

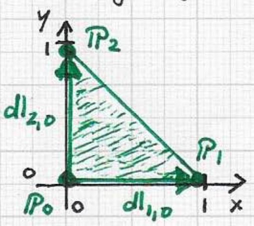
OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

• Laplacian eigenfunctions: ... The volumes of the 3 sub-triangles are:

$$v_2 = \tfrac{1}{2}\cdot 4 = 2;\ v_0 = \tfrac{1}{2}\cdot 4 = 2;\ v_1 = \tfrac{1}{2}\cdot 4 = 2.$$

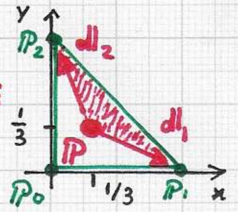
Indexing of $\mathbb{P}_0, \ldots, \mathbb{P}_{k-1}$ and location of $\mathbb{P}$ defining sign of volumes:

k = 3



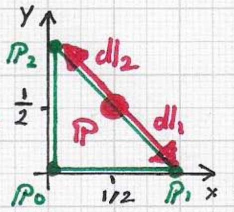
$$\begin{vmatrix} x & 1 & 0 \\ y & 0 & 1 \\ z & 0 & 0 \end{vmatrix} = 1z \Rightarrow \mathbf{n} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

INSIDE



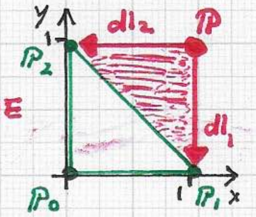
$$\begin{vmatrix} x & 2/3 & -1/3 \\ y & -1/3 & 2/3 \\ z & 0 & 0 \end{vmatrix} = \tfrac{1}{3}z \Rightarrow \mathbf{n} = \begin{pmatrix} 0 \\ 0 \\ 1/3 \end{pmatrix}$$

ON BOUNDARY



$$\begin{vmatrix} x & 1/2 & -1/2 \\ y & -1/2 & 1/2 \\ z & 0 & 0 \end{vmatrix} = 0z \Rightarrow \mathbf{n}_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

OUTSIDE



$$\begin{vmatrix} x & 0 & -1 \\ y & -1 & 0 \\ z & 0 & 0 \end{vmatrix} = -1z \Rightarrow \mathbf{n}_0 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$$

The normal of the "reference triangle" defines the + OUTWARD direction; the outward normal is $(0,0,1)^T$.

Three scenarios are shown for normal $\mathbf{n}_0$ of the sub-triangle $\mathbb{P}\mathbb{P}_1\mathbb{P}_2$. The sign of $\mathbb{P}$'s barycentric coordinate $u_0 = v_0/v$ is given by the sign of $\langle \mathbf{n}, \mathbf{n}_0 \rangle$. The shown three scenarios yield the inner product values $\frac{1}{3}$, 0 and −1.

BUT: The signs of these volumes must be determined! For this purpose one considers the angles (inner product values) between $\mathbf{n}$ and $\mathbf{n}_2$, $\mathbf{n}$ and $\mathbf{n}_0$, and $\mathbf{n}$ and $\mathbf{n}_1$:

1) If $\langle \mathbf{n}, \mathbf{n}_i \rangle > 0$, then sign$\|\mathbf{n}_i\|$ = '+'.
2) If $\langle \mathbf{n}, \mathbf{n}_i \rangle < 0$, then sign$\|\mathbf{n}_i\|$ = '−'.
3) If $\langle \mathbf{n}, \mathbf{n}_i \rangle = 0$, then 'special case'.

Concerning the example, the $\langle\cdot,\cdot\rangle$ test yields:

$$\langle \mathbf{n}, \mathbf{n}_2 \rangle = -16 \Rightarrow v_2 = -2 .$$
$$\langle \mathbf{n}, \mathbf{n}_0 \rangle = 16 \Rightarrow v_0 = 2 .$$
$$\langle \mathbf{n}, \mathbf{n}_1 \rangle = 16 \Rightarrow v_1 = 2 .$$

The resulting barycentric coordinates for $\mathbb{P}$ are: $u_0 = v_0/v = 1$; $u_1 = v_1/v = 1$; $u_2 = v_2/v = -1$.

In summary, the absolute values and signs of a point's barycentric coordinates can be computed via determinants and a "simple" inner product sign test. We must apply these computations to our setting — where $\mathbb{P}$ and $\mathbb{P}_0, \ldots, \mathbb{P}_{k-1}$ are all points on a unit hyper-sphere. ...