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Exact integration for products of power of barycentric coordinates over d-simplexes in \mathbb{R}^n

François Cuvelier*

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Abstract

Exact integral computation over a d-simplex in \mathbb{R}^n for products of powers of its barycentric coordinates is done in [9] by using mathematical induction and coordinate mappings. In this note we give a new proof using Laplace transformations without mathematical induction.

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Local shape functions of a large variety of finite element on a d-simplex $K \subset \mathbb{R}^n$ can be expressed in function of the barycentric coordinates $\{\lambda_0, \dots, \lambda_d\}$ of K and their derivatives (see [1] for examples).

In [9], the authors give a proof of the *magic formula*: let $\boldsymbol{\nu} = (\nu_0, \dots, \nu_d) \in \mathbb{N}^{d+1}$, then

$$\int_K \prod_{i=0}^d \lambda_i^{\nu_i}(\mathbf{q}) d\mathbf{q} = d! |K| \frac{\prod_{i=0}^d \nu_i!}{(d + \sum_{l=0}^d \nu_l)!} \quad (1)$$

where $|K|$ is the volume of K . In their proof, mathematical induction and coordinate mappings are mainly used. In this note we give a new proof of this formula using Laplace transformations without mathematical induction.

Firstly we recall definitions of a d-simplex in \mathbb{R}^n and of its barycentric coordinates. Therafter we introduce Laplace transforms to compute the volume of the unit d-simplex $\hat{K} \subset \mathbb{R}^d$ and the *magic formula* (1) over \hat{K} . In the last section, we propose to compute the gradients of the barycentric coordinates by solving linear systems. We also present the mapping of an integral over a d-simplex in \mathbb{R}^n to the reference unit d-simplex, allowing to prove (1).

1 Notations and definitions

Let $n \in \mathbb{N}^*$ be the space dimension and $d \in \llbracket 0, n \rrbracket$. We recall the definition of a d-simplex in \mathbb{R}^n as well as its barycentric coordinates.

Definition 1 (d-simplex) *A d-simplex $K \subset \mathbb{R}^n$ is the convex hull of $(d + 1)$ points $\mathbf{q}^0, \dots, \mathbf{q}^d$ of \mathbb{R}^n which form the vertices of K .*

$$K = \left\{ \mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} = \sum_{i=0}^d \theta_i \mathbf{q}^i, \text{ with } \forall i \in \llbracket 0, d \rrbracket, \theta_i \geq 0, \text{ and } \sum_{i=0}^d \theta_i = 1 \right\}. \quad (2)$$

For example, a 2-simplex is a triangle and a 3-simplex is a tetrahedron. It will be always assumed that a d-simplex is **not degenerated**, i.e., the set of vectors $\{\mathbf{q}^i - \mathbf{q}^0\}_{i=1}^d$ is linearly independent.

Definition 2 (Barycentric coordinates) *Let $K \subset \mathbb{R}^n$ be a non-degenerate d-simplex and $\{\mathbf{q}^i\}_{i=0}^d$ its vertices. The parametrization of K with a convex combination of the vertices reads as follows*

$$K = \left\{ \mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} = \sum_{i=0}^d \lambda_i(\mathbf{q}) \mathbf{q}^i, \text{ with } \forall i \in \llbracket 0, d \rrbracket, \lambda_i(\mathbf{q}) \geq 0, \text{ and } \sum_{i=0}^d \lambda_i(\mathbf{q}) = 1 \right\}. \quad (3)$$

The coefficients $\lambda_0(\mathbf{q}), \dots, \lambda_d(\mathbf{q})$ are called the barycentric coordinates on K of \mathbf{q} .

As immediat property, the barycentric coordinates on K satisfy

$$\lambda_i(\mathbf{q}^j) = \delta_{i,j}, \quad \forall (i, j) \in \llbracket 0, d \rrbracket. \quad (4)$$

2 Some results on the unit d-simplex

The **unit d-simplex** $\hat{K}^d \subset \mathbb{R}^d$ is defined by the $d + 1$ vertices

$$\{\hat{\mathbf{q}}^0, \hat{\mathbf{q}}^1, \dots, \hat{\mathbf{q}}^d\} = \{\mathbf{0}, \hat{\mathbf{e}}^1, \dots, \hat{\mathbf{e}}^d\}$$

where $\{\hat{\mathbf{e}}^1, \dots, \hat{\mathbf{e}}^d\}$ is the standard basis of \mathbb{R}^d . We have

$$\hat{K}^d = \left\{ \hat{\mathbf{q}} \in \mathbb{R}^d \mid \hat{\mathbf{q}} = \sum_{i=0}^d \hat{\lambda}_i(\hat{\mathbf{q}}) \hat{\mathbf{q}}^i, \text{ with } \hat{\lambda}_i(\hat{\mathbf{q}}) \geq 0, \text{ and } \sum_{i=0}^d \hat{\lambda}_i(\hat{\mathbf{q}}) = 1 \right\}. \quad (5)$$

As immediat property, the barycentric coordinates $(\hat{\lambda}_i)_{i=0}^d$ on \hat{K}^d satisfy

$$\hat{\lambda}_i(\hat{\mathbf{q}}^j) = \delta_{i,j}, \quad \forall (i, j) \in \llbracket 0, d \rrbracket. \quad (6)$$

and are explicitly given with $\hat{\mathbf{q}} = (x_1, \dots, x_d)^\mathbf{t} \in \hat{K}^d$ by

$$\hat{\lambda}_0(\hat{\mathbf{q}}) = 1 - \sum_{i=1}^d x_i \quad \text{and } \forall i \in \llbracket 1, d \rrbracket, \quad \hat{\lambda}_i(\hat{\mathbf{q}}) = x_i. \quad (7)$$

Indeed, as $\hat{\mathbf{q}}^0 = \mathbf{0}$, we have

$$\hat{\mathbf{q}} = \sum_{i=0}^d \hat{\lambda}_i(\hat{\mathbf{q}}) \hat{\mathbf{q}}^i = \sum_{i=1}^d \hat{\mathbf{q}}^i \hat{\lambda}_i(\hat{\mathbf{q}})$$

From $\hat{\mathbf{q}}^i = \hat{\mathbf{e}}^i$, $\forall i \in \llbracket 1, d \rrbracket$, we obtain

$$\sum_{i=1}^d \hat{\mathbf{q}}^i \hat{\lambda}_i(\hat{\mathbf{q}}) = \begin{pmatrix} \hat{\mathbf{q}}^1 & \cdots & \hat{\mathbf{q}}^d \\ \vdots & & \vdots \end{pmatrix} \begin{pmatrix} \hat{\lambda}_1(\hat{\mathbf{q}}) \\ \vdots \\ \hat{\lambda}_d(\hat{\mathbf{q}}) \end{pmatrix} = \mathbb{1}_d \begin{pmatrix} \hat{\lambda}_1(\hat{\mathbf{q}}) \\ \vdots \\ \hat{\lambda}_d(\hat{\mathbf{q}}) \end{pmatrix} = \begin{pmatrix} \hat{\lambda}_1(\hat{\mathbf{q}}) \\ \vdots \\ \hat{\lambda}_d(\hat{\mathbf{q}}) \end{pmatrix}$$

and thus

$$\hat{\mathbf{q}} = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} = \begin{pmatrix} \hat{\lambda}_1(\hat{\mathbf{q}}) \\ \vdots \\ \hat{\lambda}_d(\hat{\mathbf{q}}) \end{pmatrix}.$$

From (5), we have

$$\sum_{i=0}^d \hat{\lambda}_i(\hat{\mathbf{q}}) = 1$$

and thus

$$\hat{\lambda}_0(\hat{\mathbf{q}}) = 1 - \sum_{i=1}^d \hat{\lambda}_i(\hat{\mathbf{q}}) = 1 - \sum_{i=1}^d x_i.$$

2.1 unit d-simplex volume

There are several ways to compute the volume $|\hat{K}|$ of the d-simplex $\hat{K} \subset \mathbb{R}^d$ which is given by the following integral:

$$|\hat{K}| = \int_{\hat{K}} 1 d\hat{\mathbf{q}} = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \cdots \int_0^{1-(x_1+\dots+x_{d-1})} 1 dx_d \dots dx_3 dx_2 dx_1.$$

An elegant way to perform this integration is explained in [6], section 18.10, and uses a Laplace transform. To use this method, we note that

$$\hat{K} = \mathbb{R}_+^d \cap \{1 - (x_1 + \dots + x_d) \geq 0\}. \quad (8)$$

So we also have

$$|\hat{K}| = \int_{\mathbb{R}_+^d \cap \{1 - (x_1 + \dots + x_d) \geq 0\}} 1 dx_d \dots dx_1.$$

By using a dirac function and extending the integration domain to \mathbb{R}_+^{d+1} , we also have

$$|\hat{K}| = \int_{\mathbb{R}_+^{d+1}} \delta(x_1 + \dots + x_d + x_{d+1} - 1) dx_{d+1} dx_d \dots dx_1$$

To use the Laplace transform theory, we define the function f by

$$f(t) = \int_{\mathbb{R}_+^{d+1}} \delta(x_1 + \dots + x_d + x_{d+1} - t) dx_{d+1} dx_d \dots dx_1$$

so that $|\hat{K}| = f(1)$. The Laplace transform of f is given by

$$\begin{aligned} \mathcal{L}(f)(s) &= \int_0^\infty f(t) e^{-st} dt \\ &= \int_{\mathbb{R}_+^{d+1}} \left(\int_0^\infty \delta(x_1 + \dots + x_d + x_{d+1} - t) e^{-st} dt \right) dx_{d+1} dx_d \dots dx_1 \\ &= \int_{\mathbb{R}_+^{d+1}} \exp\left(-s \sum_{i=1}^{d+1} x_i\right) dx_{d+1} dx_d \dots dx_1 \\ &= \prod_{i=1}^{d+1} \int_0^\infty \exp(-sx_i) dx_i \\ &= \frac{1}{s^{d+1}}. \end{aligned}$$

By using the inverse Laplace transform table (see [8] for example), we have

$$\mathcal{L}^{-1}\left(s \mapsto \frac{d!}{s^{d+1}}\right)(t) = t^d.$$

As $f = \mathcal{L}^{-1} \circ \mathcal{L}(f)$ and by linearity of the inverse Laplace transform we obtain

$$f(t) = \frac{t^d}{d!}.$$

So the volume of the unit d -simplex is

$$|\hat{K}| = \frac{1}{d!} \quad (9)$$

2.2 Magic formula

Let $\boldsymbol{\nu} = (\nu_0, \dots, \nu_d) \in \mathbb{N}^{d+1}$. The *magic formula* is given by

$$\int_{\hat{K}} \prod_{i=0}^d \hat{\lambda}_i^{\nu_i}(\hat{\mathbf{q}}) d\hat{\mathbf{q}} = \frac{\prod_{i=0}^d \nu_i!}{(d + \sum_{i=0}^d \nu_i)!} \quad (10)$$

This formula is often used in \mathbb{P}^1 -Lagrange finite element methods because \mathbb{P}^1 -Lagrange basis functions on a d -simplex are the associated barycentric coordinates. For example, one can refer to [7] (section 8.2.1, page 179, formula (8.3)), [9], [4] section 7.3.3 page 126, [3] for $d \in \llbracket 1, 3 \rrbracket$, [2] as exercise for $d = 2$ and $d = 3$. In this section, we propose a proof of this formula using Laplace transform theory. Let $\hat{I}(\boldsymbol{\nu})$ denote the integral of (10). The barycentric coordinates $\hat{\lambda}_i$ are given in (7) and so with $\hat{\mathbf{q}} = (x_1, \dots, x_d)$ and using (8) we obtain

$$\begin{aligned} \hat{I}(\boldsymbol{\nu}) &= \int_{\hat{K}} (1 - \sum_{i=1}^d x_i)^{\nu_0} \prod_{i=1}^d x_i^{\nu_i} dx_d \dots dx_1 \\ &= \int_{\mathbb{R}_+^d \cap \{1 - (x_1 + \dots + x_d) \geq 0\}} (1 - \sum_{i=1}^d x_i)^{\nu_0} \prod_{i=1}^d x_i^{\nu_i} dx_d \dots dx_1 \end{aligned}$$

From section 2.1, by using a dirac function and by extending the integration domain to \mathbb{R}_+^{d+1} we obtain with $\nu_{d+1} = \nu_0$

$$\begin{aligned} \hat{I}(\boldsymbol{\nu}) &= \int_{\mathbb{R}_+^{d+1}} \delta(x_1 + \dots + x_d + x_{d+1} - 1) x_{d+1}^{\nu_0} \prod_{i=1}^d x_i^{\nu_i} dx_{d+1} dx_d \dots dx_1 \\ &= \int_{\mathbb{R}_+^{d+1}} \delta(x_1 + \dots + x_d + x_{d+1} - 1) \prod_{i=1}^{d+1} x_i^{\nu_i} dx_{d+1} dx_d \dots dx_1 \end{aligned}$$

To use the Laplace transform theory, we define the function $f_{\boldsymbol{\nu}}$ by

$$f_{\boldsymbol{\nu}}(t) = \int_{\mathbb{R}_+^{d+1}} \delta(x_1 + \dots + x_d + x_{d+1} - t) \prod_{i=1}^{d+1} x_i^{\nu_i} dx_{d+1} dx_d \dots dx_1$$

so that $\hat{I}(\boldsymbol{\nu}) = f_{\boldsymbol{\nu}}(1)$. The Laplace transform of $f_{\boldsymbol{\nu}}$ is given by

$$\begin{aligned} \mathcal{L}(f_{\boldsymbol{\nu}})(s) &= \int_0^\infty f_{\boldsymbol{\nu}}(t) e^{-st} dt \\ &= \int_{\mathbb{R}_+^{d+1}} \left(\int_0^\infty \delta(x_1 + \dots + x_d + x_{d+1} - t) e^{-st} dt \right) \prod_{i=1}^{d+1} x_i^{\nu_i} dx_{d+1} dx_d \dots dx_1 \\ &= \int_{\mathbb{R}_+^{d+1}} \exp(-s \sum_{i=1}^{d+1} x_i) \prod_{i=1}^{d+1} x_i^{\nu_i} dx_{d+1} dx_d \dots dx_1 \\ &= \prod_{i=1}^{d+1} \int_0^\infty x_i^{\nu_i} \exp(-s x_i) dx_i \\ &= \prod_{i=1}^{d+1} \mathcal{L}(t \mapsto t^{\nu_i})(s) \end{aligned}$$

In a classical Laplace transform table (see [8] for example), we have

$$\mathcal{L}(t \mapsto \frac{t^k}{k!})(s) = \frac{1}{s^{k+1}}$$

and by linearity of the Laplace transform

$$\mathcal{L}(t \mapsto t^k)(s) = \frac{k!}{s^{k+1}}.$$

So we obtain

$$\mathcal{L}(f_{\boldsymbol{\nu}})(s) = \prod_{i=1}^{d+1} \frac{\nu_i!}{s^{\nu_i+1}} = \frac{\prod_{i=1}^{d+1} \nu_i!}{s^{d+1+\sum_{i=1}^{d+1} \nu_i}}$$

By using the inverse Laplace transform table, we have

$$\mathcal{L}^{-1}(s \mapsto \frac{1}{s^k})(t) = \frac{t^{k-1}}{k-1}.$$

With the linearity of the inverse Laplace transform we obtain

$$\begin{aligned} f_{\boldsymbol{\nu}}(t) &= \mathcal{L}^{-1}(\mathcal{L}(f_{\boldsymbol{\nu}})(s))(t) \\ &= \frac{\prod_{i=1}^{d+1} \nu_i!}{(d + \sum_{i=1}^{d+1} \nu_i)!} t^{d+\sum_{i=1}^{d+1} \nu_i}. \end{aligned}$$

As $\hat{I}(\nu) = f_{\boldsymbol{\nu}}(1)$ and $\nu_{d+1} = \nu_0$, the equation (10) is proved.

3 Some results on a d-simplex in \mathbb{R}^n

3.1 Gradients of Barycentric coordinates on a d-simplex

Lemma 3 *Let $K \subset \mathbb{R}^n$ be a non-degenerate d-simplex and and $\{\mathbf{q}^i\}_{i=0}^d$ its vertices. The barycentric coordinates $(\lambda_i(\mathbf{q}))_{i=0}^d$ are solution of the linear system*

$$\left(\begin{array}{c|ccc} 1 & 1 & \cdots & 1 \\ \hline 0 & & & \\ \vdots & & \mathbb{A}_K^t \mathbb{A}_K & \\ 0 & & & \end{array} \right) \begin{pmatrix} \lambda_0(\mathbf{q}) \\ \lambda_1(\mathbf{q}) \\ \vdots \\ \lambda_d(\mathbf{q}) \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ \mathbb{A}_K(\mathbf{q} - \mathbf{q}^0) \end{pmatrix} \quad (11)$$

where $\mathbb{A}_K \in \mathcal{M}_{n,d}(\mathbb{R})$ is defined by

$$\mathbb{A}_K = \left(\begin{array}{c|ccc} & \vdots & & \vdots \\ \mathbf{q}^1 - \mathbf{q}^0 & & \cdots & \\ \vdots & & & \\ \mathbf{q}^d - \mathbf{q}^0 & & & \end{array} \right) \quad (12)$$

The barycentric coordinates are multivariate polynomials of first degree and their gradients are given by

$$\left(\nabla \lambda_1(\mathbf{q}) \quad \vdots \quad \cdots \quad \vdots \quad \nabla \lambda_d(\mathbf{q}) \right) = \mathbb{A}_K (\mathbb{A}_K^t \mathbb{A}_K)^{-1} \quad (13)$$

and

$$\nabla \lambda_0(\mathbf{q}) = - \sum_{i=1}^d \nabla \lambda_i(\mathbf{q}). \quad (14)$$

Proof: As $\sum_{i=0}^d \lambda_i(\mathbf{q}) = 1$, we have

$$\mathbf{q} = \sum_{i=0}^d \lambda_i(\mathbf{q}) \mathbf{q}^i \implies \mathbf{q} - \mathbf{q}^0 = \sum_{i=1}^d (\mathbf{q}^i - \mathbf{q}^0) \lambda_i(\mathbf{q}) = \mathbb{A}_K \begin{pmatrix} \lambda_1(\mathbf{q}) \\ \vdots \\ \lambda_d(\mathbf{q}) \end{pmatrix}$$

Due to linear independence of $\{\mathbf{q}^i - \mathbf{q}^0\}_{i=1}^d$,

$$\mathbb{H}_K \stackrel{\text{def}}{=} \mathbb{A}_K^t \mathbb{A}_K \in \mathcal{M}_{d,d}(\mathbb{R}) \quad (15)$$

is a regular matrix and the barycentric coordinates are solution of the linear system

$$\mathbb{A}_K^t \mathbb{A}_K \begin{pmatrix} \lambda_1(\mathbf{q}) \\ \vdots \\ \lambda_d(\mathbf{q}) \end{pmatrix} = \mathbb{A}_K^t (\mathbf{q} - \mathbf{q}^0) \quad \text{and} \quad \sum_{i=0}^d \lambda_i(\mathbf{q}) = 1.$$

In matrix form these equations can be written as (11) and we deduce that the barycentric coordinates λ_i are multivariate polynomials of first degree. So their gradients are constants on K .

The affine map/transformation \mathcal{F}_K from the unit d-simplex $\hat{K} \subset \mathbb{R}^d$ to $K \subset \mathbb{R}^n$ is given by

$$\mathbf{q} = \mathbb{A}_K \hat{\mathbf{q}} + \mathbf{q}^0 = \mathcal{F}_K(\hat{\mathbf{q}}). \quad (16)$$

So we have

$$\mathbb{A}_K^t (\mathbf{q} - \mathbf{q}^0) = \mathbb{A}_K^t \mathbb{A}_K \hat{\mathbf{q}} = \mathbb{H}_K \hat{\mathbf{q}}$$

and thus $\mathcal{F}_K^{-1} : K \subset \mathbb{R}^n \longrightarrow \hat{K} \subset \mathbb{R}^d$ is defined by

$$\hat{\mathbf{q}} = \mathbb{H}_K^{-1} \mathbb{A}_K^t (\mathbf{q} - \mathbf{q}^0) = \mathcal{F}_K^{-1}(\mathbf{q}). \quad (17)$$

So we have

$$\lambda_i(\mathbf{q}) = (\hat{\lambda}_i \circ \mathcal{F}_K^{-1})(\mathbf{q}) \quad \text{and} \quad \hat{\lambda}_i(\hat{\mathbf{q}}) = (\lambda_i \circ \mathcal{F}_K)(\hat{\mathbf{q}}) \quad (18)$$

One can remark that if $d = n$ then \mathbb{A}_K is a regular square matrix and $\mathbb{H}_K^{-1} \mathbb{A}_K^t = \mathbb{A}_K^{-1}$.

Now, we may compute partial derivative of λ_i and $\forall i \in \llbracket 0, d \rrbracket$, $\forall j \in \llbracket 1, n \rrbracket$, we obtain with $\hat{\mathbf{q}} = (\hat{x}_1, \dots, \hat{x}_d)$ and $\mathbf{q} = (x_1, \dots, x_n)$

$$\frac{\partial \lambda_i}{\partial x_j}(\mathbf{q}) = \sum_{l=1}^d \frac{\partial \hat{\lambda}_i}{\partial \hat{x}_j}(\mathcal{F}_K^{-1}(\mathbf{q})) \frac{\partial \mathcal{F}_K^{-1,l}}{\partial x_j}(\mathbf{q})$$

From (17), denoting $\mathbb{B}_K = \mathbb{H}_K^{-1} \mathbb{A}_K^t \in \mathcal{M}_{d,m}(\mathbb{R})$ gives $\frac{\partial \mathcal{F}_K^{-1,l}}{\partial x_j}(\mathbf{q}) = (\mathbb{B}_K)_{l,j}$. The barycentric coordinates are polynomials of first degree, so their gradients are constants and we obtain

$$\nabla \lambda_i = \mathbb{B}_K^t \hat{\nabla} \hat{\lambda}_i$$

(in fact \mathbb{B}_K is the Jacobian matrix of \mathcal{F}_K^{-1}). The matrix \mathbb{H}_K is regular and symmetric, so $\mathbb{B}_K^t = \mathbb{A}_K \mathbb{H}_K^{-1}$ and we obtain

$$\nabla \lambda_i = \mathbb{A}_K \mathbb{H}_K^{-1} \hat{\nabla} \hat{\lambda}_i. \quad (19)$$

From (7), we deduced that

$$\left(\hat{\nabla}\hat{\lambda}_1 \mid \cdots \mid \hat{\nabla}\hat{\lambda}_d \right) = \mathbb{1}_d \quad (20)$$

and thus

$$\begin{aligned} \left(\nabla\lambda_1(\mathbf{q}) \mid \cdots \mid \nabla\lambda_d(\mathbf{q}) \right) &= \mathbb{A}_K \mathbb{H}_K^{-1} \left(\hat{\nabla}\hat{\lambda}_1 \mid \cdots \mid \hat{\nabla}\hat{\lambda}_d \right) \\ &= \mathbb{A}_K \mathbb{H}_K^{-1}. \end{aligned}$$

As $\sum_{i=0}^d \lambda_i(\mathbf{q}) = 1$, we immediately have

$$\nabla\lambda_0(\mathbf{q}) = - \sum_{i=1}^d \nabla\lambda_i(\mathbf{q}).$$

□

From (13) and (14), we immediatly have:

Remark 4 *The gradients of the barycentric coordinates are linear combinations of $\{\mathbf{q}^1 - \mathbf{q}^0, \dots, \mathbf{q}^d - \mathbf{q}^0\}$.*

3.2 Integration over a d -simplex

If K is a non-degenerated d -simplex in \mathbb{R}^d , from (16) we have $\mathcal{F}_{\mathcal{F}_K}(\hat{\mathbf{q}}) = \mathbb{A}_K$. Then \mathbb{A}_K is a regular **square** matrix and we have the classical formula:

$$\int_K f(\mathbf{q}) d\mathbf{q} = |\det(\mathbb{A}_K)| \int_{\hat{K}} f \circ \mathcal{F}_K(\hat{\mathbf{q}}) d\hat{\mathbf{q}} \quad (21)$$

The following theorem extend this result to d -simplex in \mathbb{R}^n , with $1 \leq d \leq n$.

Theorem 5 *Let $K \subset \mathbb{R}^n$ be a non-degenerated d -simplex and $f : K \rightarrow \mathbb{R}$.*

$$\int_K f(\mathbf{q}) d\mathbf{q} = |\det(\mathbb{A}_K^{\dagger} \mathbb{A}_K)|^{1/2} \int_{\hat{K}} f \circ \mathcal{F}_K(\hat{\mathbf{q}}) d\hat{\mathbf{q}} \quad (22)$$

where K is the unit d -simplex in \mathbb{R}^n , $\mathbb{A}_K \in \mathcal{M}_{d,n}(\mathbb{R})$ is defined by

$$\mathbb{A}_K = \left(\mathbf{q}^1 - \mathbf{q}^0 \mid \mathbf{q}^2 - \mathbf{q}^0 \mid \cdots \mid \mathbf{q}^d - \mathbf{q}^0 \right) \quad (23)$$

and $\mathcal{F}_K : \hat{K} \rightarrow K$ is given by

$$\mathcal{F}_K(\hat{\mathbf{q}}) = \mathbb{A}_K \hat{\mathbf{q}} + \mathbf{q}^0 \quad (24)$$

Proof: The set $\{\mathbf{v}^1, \dots, \mathbf{v}^d\}$ is linearly independent so we can extend it to a basis $\{\mathbf{v}^1, \dots, \mathbf{v}^n\}$. We denote by $\mathbb{A} \in \mathcal{M}_{n,n}(\mathbb{R})$ the matrix such that the i -th column is the vector \mathbf{v}^i for all $i \in \llbracket 1, n \rrbracket$. So we have

$$\mathbb{A} = \left(\mathbb{A}_K \mid \mathbf{v}^{d+1} \mid \cdots \mid \mathbf{v}^n \right) \quad (25)$$

By the QR-factorization theorem apply to the matrix $\mathbb{A} \in \mathcal{M}_n(\mathbb{R})$, there is an orthogonal matrix $\mathbb{Q} \in \mathcal{M}_n(\mathbb{R})$ and a regular upper triangular matrix $\mathbb{R} \in \mathcal{M}_n(\mathbb{R})$ such that

$$\mathbb{A} = \mathbb{Q}\mathbb{R}$$

So we have

$$\mathbb{Q}^t \mathbb{A} = \mathbb{R}$$

and we define the matrix $\bar{\mathbb{A}} \in \mathcal{M}_{n,d}(\mathbb{R})$ to be the first d columns of \mathbb{R} :

$$\bar{\mathbb{A}} = \mathbb{Q}^t \mathbb{A}_K.$$

We can also note that

$$\bar{\mathbb{A}} = \left(\bar{\mathbf{q}}^1 - \bar{\mathbf{q}}^0 \mid \bar{\mathbf{q}}^2 - \bar{\mathbf{q}}^0 \mid \cdots \mid \bar{\mathbf{q}}^d - \bar{\mathbf{q}}^0 \right) = \left(\bar{\mathbf{q}}^1 \mid \bar{\mathbf{q}}^2 \mid \cdots \mid \bar{\mathbf{q}}^d \right).$$

Let $\bar{\mathcal{F}} : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ be the bijective function defined by

$$\bar{\mathcal{F}}(\mathbf{x}) = \mathbb{Q}^t(\mathbf{x} - \mathbf{q}^0) = \bar{\mathbf{x}} \quad (26)$$

and

$$\bar{\mathbf{q}}^i = \bar{\mathcal{F}}(\mathbf{q}^i) = \mathbb{Q}^t(\mathbf{q}^i - \mathbf{q}^0), \quad \forall i \in \llbracket 0, d \rrbracket.$$

By construction $\bar{\mathbf{q}}^0 = \mathbf{0}$ and, $\forall i \in \llbracket 1, d \rrbracket$, $\bar{\mathbf{q}}^i$ is the i -th column of the upper triangular matrix \mathbb{R} . So we have

$$\forall i \in \llbracket 0, d \rrbracket, \quad \bar{\mathbf{q}}^i \in \text{Vect}(\mathbf{e}^1, \dots, \mathbf{e}^d)$$

where $\{\mathbf{e}^1, \dots, \mathbf{e}^d\}$ is the standard basis of \mathbb{R}^n . The set $\{\bar{\mathbf{q}}^0, \dots, \bar{\mathbf{q}}^d\}$ are the vertices of the d -simplex $\bar{K} = \bar{\mathcal{F}}(K)$ and we deduce

$$\bar{K} \subset \text{Vect}(\mathbf{e}^1, \dots, \mathbf{e}^d). \quad (27)$$

By change of variables, we obtain

$$\int_K f(\mathbf{q}) d\mathbf{q} = \int_{\bar{K}} f \circ \bar{\mathcal{F}}^{-1}(\bar{\mathbf{q}}) |\det(\mathcal{J}_{\bar{\mathcal{F}}^{-1}}(\bar{\mathbf{q}}))| d\bar{\mathbf{q}}$$

where $\mathcal{J}_{\bar{\mathcal{F}}^{-1}}$ is the Jacobian matrix of $\bar{\mathcal{F}}^{-1}$. From (26), we have $\mathcal{J}_{\bar{\mathcal{F}}^{-1}}(\bar{\mathbf{q}}) = \mathbb{Q}$ and as \mathbb{Q} is an orthogonal matrix, $\det(\mathcal{J}_{\bar{\mathcal{F}}^{-1}}(\bar{\mathbf{q}})) = 1$. So we obtain

$$\int_K f(\mathbf{q}) d\mathbf{q} = \int_{\bar{K}} f \circ \bar{\mathcal{F}}^{-1}(\bar{\mathbf{q}}) d\bar{\mathbf{q}}. \quad (28)$$

Let $\mathbb{P} \in \mathcal{M}_{d,n}(\mathbb{R})$ defined by

$$\mathbb{P} = \left(\mathbb{1}_d \mid \mathbb{0}_{d,n-d} \right)$$

and

$$\forall i \in \llbracket 0, d \rrbracket, \quad \bar{\bar{\mathbf{q}}}^i = \mathbb{P} \bar{\mathbf{q}}^i \in \mathbb{R}^d.$$

From (27), we deduce

$$\forall i \in \llbracket 0, d \rrbracket, \quad \bar{\bar{\mathbf{q}}}^i = \mathbb{P}^t \bar{\mathbf{q}}^i = \begin{pmatrix} \bar{\bar{\mathbf{q}}}^i \\ \mathbf{0} \end{pmatrix}.$$

Let $\bar{g} = f \circ \bar{\mathcal{F}}^{-1}$ and $\bar{\bar{K}}$ be the d -simplex in \mathbb{R}^d with vertices $\bar{\bar{\mathbf{q}}}^i$, $i \in \llbracket 0, d \rrbracket$. We denote by $\mathcal{P} : \bar{\bar{K}} \subset \mathbb{R}^d \longrightarrow \bar{K} \subset \mathbb{R}^n$ the application defined by $\mathcal{P}(\bar{\bar{\mathbf{q}}}) = \mathbb{P}^t \bar{\bar{\mathbf{q}}}$. We denote by $\bar{\bar{g}} : \bar{\bar{K}} \longrightarrow \mathbb{R}$ the application defined by

$$\bar{\bar{g}}(\bar{\bar{\mathbf{q}}}) = \bar{g} \circ \mathcal{P}(\bar{\bar{\mathbf{q}}}) = \bar{g} \left(\begin{pmatrix} \bar{\bar{\mathbf{q}}} \\ \mathbf{0} \end{pmatrix} \right).$$

So we obtain

$$\int_{\bar{K}} \bar{g}(\bar{\mathbf{q}}) d\bar{\mathbf{q}} = \int_{\bar{K}} \bar{g}(\bar{\mathbf{q}}) d\bar{\mathbf{q}} \quad (29)$$

Let $\bar{\bar{A}} \in \mathcal{M}_d(\mathbb{R})$ be the matrix defined by

$$\bar{\bar{A}} = \begin{pmatrix} \bar{\mathbf{q}}^1 - \bar{\mathbf{q}}^0 & \bar{\mathbf{q}}^2 - \bar{\mathbf{q}}^0 & \dots & \bar{\mathbf{q}}^d - \bar{\mathbf{q}}^0 \end{pmatrix}. \quad (30)$$

We can remark that

$$\bar{\bar{A}} = \mathbb{P} \bar{A} \quad \text{and} \quad \bar{A} = \mathbb{P}^t \bar{\bar{A}}.$$

Let $\bar{\bar{F}} : \hat{K} \rightarrow \bar{K}$ the bijective function defined by

$$\bar{\bar{F}}(\hat{\mathbf{q}}) = \bar{\bar{A}} \hat{\mathbf{q}} + \bar{\mathbf{q}}^0$$

We can now apply the classical change of variables

$$\begin{aligned} \int_{\bar{K}} \bar{g}(\bar{\mathbf{q}}) d\bar{\mathbf{q}} &= \int_{\hat{K}} \bar{g} \circ \bar{\bar{F}}(\hat{\mathbf{q}}) |\det(\mathcal{J}_{\bar{\bar{F}}}(\hat{\mathbf{q}}))| d\hat{\mathbf{q}} \\ &= |\det(\bar{\bar{A}})| \int_{\hat{K}} \bar{g} \circ \bar{\bar{F}}(\hat{\mathbf{q}}) d\hat{\mathbf{q}} \end{aligned}$$

To resume from (22) and (29), we have

$$\int_K f(\mathbf{q}) d\mathbf{q} = |\det(\bar{\bar{A}})| \int_{\hat{K}} \bar{g} \circ \bar{\bar{F}}(\hat{\mathbf{q}}) d\hat{\mathbf{q}} \quad (31)$$

We can note that

$$\bar{g} \circ \bar{\bar{F}} = f \circ \bar{F}^{-1} \circ \mathcal{P} \circ \bar{F}$$

Let $\mathcal{F}_K = \bar{F}^{-1} \circ \mathcal{P} \circ \bar{F}$, we have as expected

$$\begin{aligned} \mathcal{F}_K(\hat{\mathbf{q}}) &= \bar{F}^{-1} \circ \mathcal{P} \circ \bar{F}(\hat{\mathbf{q}}) \\ &= \bar{F}^{-1}(\mathbb{P}^t(\bar{\bar{A}}\hat{\mathbf{q}})) \\ &= \bar{F}^{-1}(\bar{A}\hat{\mathbf{q}}) \\ &= \mathbb{Q}\bar{A}\hat{\mathbf{q}} + \mathbf{q}^0 \\ &= \mathbb{A}_K\hat{\mathbf{q}} + \mathbf{q}^0. \end{aligned}$$

and we obtain

$$\int_K f(\mathbf{q}) d\mathbf{q} = |\det(\bar{\bar{A}})| \int_{\hat{K}} f \circ \mathcal{F}_K(\hat{\mathbf{q}}) d\hat{\mathbf{q}} \quad (32)$$

To obtain formula (22), it remains to prove that $|\det(\bar{\bar{A}})| = |\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2}$.

We have

$$\begin{aligned} \mathbb{A}_K^t \mathbb{A}_K &= \mathbb{A}_K^t \mathbb{Q} \mathbb{Q}^t \mathbb{A}_K && \text{as } \mathbb{A}_K = \mathbb{Q} \bar{A} \\ &= \bar{\bar{A}}^t \bar{\bar{A}} && \text{as } \mathbb{Q} \text{ is an orthogonal matrix} \\ &= \bar{\bar{A}}^t \mathbb{P} \mathbb{P}^t \bar{\bar{A}} && \text{as } \bar{A} = \mathbb{P}^t \bar{\bar{A}} \\ &= \bar{\bar{A}}^t \bar{\bar{A}} && \text{as } \mathbb{P} \mathbb{P}^t = \mathbb{I}_d \end{aligned}$$

As $\bar{\bar{A}}$ is a square matrix, we have $\det(\bar{\bar{A}}^t \bar{\bar{A}}) = \det(\bar{\bar{A}})^2$ and thus

$$|\det(\bar{\bar{A}})| = |\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2}.$$

□

3.3 Volume of a d-simplex

The volume/measure of the d-simplex $K \subset \mathbb{R}^n$ is given by

$$|K| = \int_K 1 d\mathbf{q} \quad (33)$$

Using formula (22) with $f \equiv 1$ gives

$$|K| = |\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2} \int_{\hat{K}} 1 d\hat{\mathbf{q}} = |\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2} |\hat{K}|.$$

From (9), we finally obtain

$$|K| = \frac{|\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2}}{d!}. \quad (34)$$

In [5] this formula is proved with geometrical arguments. We can also remark that if $d \equiv n$ then \mathbb{A}_K is a square matrix and we obtain the classical formula

$$|K| = \frac{|\det(\mathbb{A}_K)|}{d!}. \quad (35)$$

3.4 Magic formula

In this section an exact computation of the integral over a d-simplex $K \subset \mathbb{R}^n$ for products of power of its barycentric coordinates given by (1) is proved by using previous results obtained by Laplace transforms.

Using formula (22) with $f(\mathbf{q}) = \prod_{i=0}^d \lambda_i^{\nu_i}(\mathbf{q})$ gives

$$\int_K \prod_{i=0}^d \lambda_i^{\nu_i}(\mathbf{q}) d\mathbf{q} = |\det(\mathbb{A}_K^t \mathbb{A}_K)|^{1/2} \int_{\hat{K}} \prod_{i=0}^d (\lambda_i \circ \mathcal{F}_K(\hat{\mathbf{q}}))^{\nu_i} d\hat{\mathbf{q}}$$

From (18) and (34), we obtain

$$\int_K \prod_{i=0}^d \lambda_i^{\nu_i}(\mathbf{q}) d\mathbf{q} = d! |K| \int_{\hat{K}} \prod_{i=0}^d \hat{\lambda}_i^{\nu_i}(\hat{\mathbf{q}}) d\hat{\mathbf{q}}$$

Using formula (10) gives (1)

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