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

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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.

Contents

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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 $\{\lambda_0, \ldots, \lambda_{\mathrm{d}}\}$ of K and their derivatives (see [1] for examples).

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

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

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 $\hat{K} \subset \mathbb{R}^{\mathrm{d}}$ 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 proove (1).

1 Notations and definitions

Let $n \in \mathbb{N}^*$ be the space dimension and $\mathrm{d} \in [\![0, n]\!]$. 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 $(\mathrm{d}+1)$ points $\mathbf{q}^0, \ldots, \mathbf{q}^{\mathrm{d}}$ of $\mathbb{R}^n$ which form the vertices of K.*

$$K = \left\{ \mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} = \sum_{i=0}^{\mathrm{d}} \theta_i \mathbf{q}^i, \ \textit{with} \ \forall i \in [\![0, \mathrm{d}]\!], \ \theta_i \geqslant 0, \ \textit{and} \ \sum_{i=0}^{\mathrm{d}} \theta_i = 1 \right\}. \tag{2}$$

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 $\{\mathbf{q}^i - \mathbf{q}^0\}_{i=1}^{\mathrm{d}}$ is linearly independent.

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

$$K = \left\{ \mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} = \sum_{i=0}^{\mathrm{d}} \lambda_i(\mathbf{q}) \mathbf{q}^i, \ \textit{with} \ \forall i \in [\![0, \mathrm{d}]\!], \ \lambda_i(\mathbf{q}) \geqslant 0, \ \textit{and} \ \sum_{i=0}^{\mathrm{d}} \lambda_i(\mathbf{q}) = 1 \right\}. \tag{3}$$

The coefficients $\lambda_0(\mathbf{q}), \ldots, \lambda_{\mathrm{d}}(\mathbf{q})$ are called the barycentric coordinates on K of $\mathbf{q}$.

As immediat property, the barycentric coordinates on K satisfy

$$\lambda_i(\mathbf{q}^j) = \delta_{i,j}, \quad \forall (i,j) \in [\![0, \mathrm{d}]\!]. \tag{4}$$

2 Some results on the unit d-simplex

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

$$\left\{\hat{\mathbf{q}}^0, \hat{\mathbf{q}}^1, \cdots, \hat{\mathbf{q}}^{\mathrm{d}}\right\} = \left\{\mathbf{0}, \hat{\boldsymbol{e}}^1, \cdots, \hat{\boldsymbol{e}}^{\mathrm{d}}\right\}$$

where $\left\{\hat{\boldsymbol{e}}^1, \ldots, \hat{\boldsymbol{e}}^{\mathrm{d}}\right\}$ is the standard basis of $\mathbb{R}^{\mathrm{d}}$. We have

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

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

$$\hat{\lambda}_i(\hat{\mathbf{q}}^j) = \delta_{i,j}, \quad \forall (i,j) \in [\![0, \mathrm{d}]\!]. \tag{6}$$

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

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

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

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

From $\hat{\mathbf{q}}^i = \hat{\boldsymbol{e}}^i, \ \forall i \in [\![1, \mathrm{d}]\!]$, we obtain

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

and thus

$$\hat{\mathbf{q}} = \begin{pmatrix} x_1 \\ \vdots \\ x_{\mathrm{d}} \end{pmatrix} = \begin{pmatrix} \hat{\lambda}_1(\hat{\mathbf{q}}) \\ \vdots \\ \hat{\lambda}_{\mathrm{d}}(\hat{\mathbf{q}}) \end{pmatrix}.$$

From (5), we have

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

and thus

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

2.1 unit d-simplex volume

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

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

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

$$\hat{K} = \mathbb{R}_+^{\mathrm{d}} \cap \{1 - (x_1 + \ldots + x_{\mathrm{d}}) \geqslant 0\}. \tag{8}$$

So we also have

$$|\hat{K}| = \int_{\mathbb{R}_+^{\mathrm{d}} \cap \{1-(x_1+\ldots+x_{\mathrm{d}})\geqslant 0\}} 1 dx_{\mathrm{d}} \ldots dx_1.$$

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

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

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

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

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

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

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

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

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

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

So the volume of the unit d-simplex is

$$|\hat{K}| = \frac{1}{\mathrm{d}!} \tag{9}$$

2.2 Magic formula

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

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

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 barycentic 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 $\mathrm{d} \in [\![1, 3]\!]$, [2] as exercise for $\mathrm{d} = 2$ and $\mathrm{d} = 3$. In this section, we propose a proof of this formula using Laplace transform theory. Let $\hat{I}(\nu)$ denote the integral of (10). The barycentic coordinates $\hat{\lambda}_i$ are given in (7) and so with $\hat{\mathbf{q}} = (x_1, \ldots, x_{\mathrm{d}})$ and using (8) we obtain

$$\begin{aligned}
\hat{I}(\nu) &= \int_{\hat{K}} (1 - \sum_{i=1}^{\mathrm{d}} x_i)^{\nu_0} \prod_{i=1}^{\mathrm{d}} x_i^{\nu_i} dx_{\mathrm{d}} \ldots dx_1 \\
&= \int_{\mathbb{R}_+^{\mathrm{d}} \cap \{1-(x_1+\ldots+x_{\mathrm{d}}) \geqslant 0\}} (1 - \sum_{i=1}^{\mathrm{d}} x_i)^{\nu_0} \prod_{i=1}^{\mathrm{d}} x_i^{\nu_i} dx_{\mathrm{d}} \ldots dx_1
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

As $\hat{I}(\nu) = f_{\boldsymbol{\nu}}(1)$ and $\nu_{\mathrm{d}+1} = \nu_0$, 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 $\{\mathbf{q}^i\}_{i=0}^{\mathrm{d}}$ its vertices. The barycentric coordinates $(\lambda_i(\mathbf{q}))_{i=0}^{\mathrm{d}}$ are solution of the linear system*

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & & & \\ \vdots & & \mathbb{A}_K^t \mathbb{A}_K & \\ 0 & & & \end{pmatrix} \begin{pmatrix} \lambda_0(\mathbf{q}) \\ \lambda_1(\mathbf{q}) \\ \vdots \\ \lambda_{\mathrm{d}}(\mathbf{q}) \end{pmatrix} = \begin{pmatrix} 1 \\ \\ \mathbb{A}_K(\mathbf{q} - \mathbf{q}^0) \\ \\ \end{pmatrix} \tag{11}$$

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

$$\mathbb{A}_K = \begin{pmatrix} \mathbf{q}^1 - \mathbf{q}^0 & \cdots & \mathbf{q}^{\mathrm{d}} - \mathbf{q}^0 \end{pmatrix} \tag{12}$$

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

$$\begin{pmatrix} \nabla \lambda_1(\mathbf{q}) & \cdots & \nabla \lambda_{\mathrm{d}}(\mathbf{q}) \end{pmatrix} = \mathbb{A}_K (\mathbb{A}_K^t \mathbb{A}_K)^{-1} \tag{13}$$

and

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

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

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

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

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

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

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

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 $\hat{K} \subset \mathbb{R}^{\mathrm{d}}$ to $K \subset \mathbb{R}^n$ is given by

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

So we have

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

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

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

So we have

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

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

Now, we may compute partial derivative of λ_i and $\forall i \in [\![0, \mathrm{d}]\!]$, $\forall j \in [\![1, n]\!]$, we obtain with $\hat{\mathbf{q}} = (\hat{x}_1, \ldots, \hat{x}_{\mathrm{d}})$ and $\mathbf{q} = (x_1, \ldots, x_n)$

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

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

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

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

$$\boldsymbol{\nabla} \lambda_i = \mathbb{A}_K \mathbb{H}_K^{-1} \hat{\boldsymbol{\nabla}} \hat{\lambda}_i. \tag{19}$$

From (7), we deduced that

$$\left(\hat{\nabla}\hat{\lambda}_1 \,\vdots\, \cdots \,\vdots\, \hat{\nabla}\hat{\lambda}_{\mathrm{d}} \right) = \mathbb{I}_{\mathrm{d}} \tag{20}$$

and thus

$$\begin{aligned} \left(\nabla \lambda_1(\mathbf{q}) \,\vdots\, \cdots \,\vdots\, \nabla \lambda_{\mathrm{d}}(\mathbf{q}) \right) &= \mathbb{A}_K \mathbb{H}_K^{-1} \left(\hat{\nabla}\hat{\lambda}_1 \,\vdots\, \cdots \,\vdots\, \hat{\nabla}\hat{\lambda}_{\mathrm{d}} \right) \\ &= \mathbb{A}_K \mathbb{H}_K^{-1}. \end{aligned}$$

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

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

□

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

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

3.2 Integration over a d-simplex

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

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

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

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

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

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

$$\mathbb{A}_K = \left(\mathbf{q}^1 - \mathbf{q}^0 \,\vdots\, \mathbf{q}^2 - \mathbf{q}^0 \,\vdots\, \cdots \,\vdots\, \mathbf{q}^{\mathrm{d}} - \mathbf{q}^0 \right) \tag{23}$$

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

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

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

$$\mathbb{A} = \left(\mathbb{A}_K \,\vdots\, \boldsymbol{v}^{\mathrm{d}+1} \,\vdots\, \cdots \,\vdots\, \boldsymbol{v}^n \right) \tag{25}$$

By the $\mathbb{QR}$-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

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

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

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

We can also note that

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

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

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

and

$$\bar{\mathbf{q}}^i = \bar{\mathcal{F}}(\mathbf{q}^i) = \mathbb{Q}^{\mathsf{t}}(\mathbf{q}^i - \mathbf{q}^0), \quad \forall i \in [\![0, \mathrm{d}]\!].$$

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

$$\forall i \in [\![0, \mathrm{d}]\!], \quad \bar{\mathbf{q}}^i \in \mathrm{Vect}(\boldsymbol{e}^1, \ldots, \boldsymbol{e}^{\mathrm{d}})$$

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

$$\bar{K} \subset \mathrm{Vect}(\boldsymbol{e}^1, \ldots, \boldsymbol{e}^{\mathrm{d}}). \tag{27}$$

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

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

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

$$\mathbb{P} = \left(\mathbb{I}_d \,\vdots\, \mathbb{O}_{d,n-d} \right)$$

and

$$\forall i \in [\![0, \mathrm{d}]\!], \quad \bar{\bar{\mathbf{q}}}^i = \mathbb{P}\bar{\mathbf{q}}^i \in \mathbb{R}^{\mathrm{d}}.$$

From (27), we deduce

$$\forall i \in [\![0, \mathrm{d}]\!], \quad \bar{\mathbf{q}}^i = \mathbb{P}^{\mathsf{t}}\bar{\bar{\mathbf{q}}}^i = \begin{pmatrix} \bar{\bar{\mathbf{q}}}^i \\ \hdashline \mathbf{0} \end{pmatrix}.$$

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

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

So we obtain

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

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

$$\bar{\bar{\mathbb{A}}} = \left(\begin{array}{c:c:c:c} \bar{\bar{\mathbf{q}}}^1 - \bar{\bar{\mathbf{q}}}^0 & \bar{\bar{\mathbf{q}}}^2 - \bar{\bar{\mathbf{q}}}^0 & \cdots & \bar{\bar{\mathbf{q}}}^{\mathrm{d}} - \bar{\bar{\mathbf{q}}}^0 \end{array} \right). \tag{30}$$

We can remark that

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

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

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

We can now apply the classical change of variables

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

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

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

We can note that

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

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

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

and we obtain

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

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

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

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

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

□

3.3 Volume of a d-simplex

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

$$|K| = \int_K 1 d\mathbf{q} \tag{33}$$

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

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

From (9), we finally obtain

$$|K| = \frac{\left|\det(\mathbb{A}_K^{\mathsf{t}} \mathbb{A}_K)\right|^{1/2}}{\mathrm{d}!}. \tag{34}$$

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

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

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 $f(\mathbf{q}) = \prod_{i=0}^{\mathrm{d}} \lambda_i^{\nu_i}(\mathbf{q})$ gives

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

From (18) and (34), we obtain

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

Using formula (10) gives (1)

References

[1] Douglas N. Arnold, Richard S. Falk, and Ragnar Winther. Geometric decompositions and local bases for spaces of finite element differential forms. *Computer Methods in Applied Mechanics and Engineering*, 198(21):1660 – 1672, 2009. Advances in Simulation-Based Engineering Sciences – Honoring J. Tinsley Oden.

[2] Susanne C. Brenner and L. Ridgway Scott. *The Mathematical Theory of Finite Element Methods*. Texts in Applied Mathematics. Springer, New York, Berlin, Paris, 2008.

[3] M.A. Eisenberg and L. E. Malvern. On finite element integration in natural co-ordinates. *Int. J. Numer. Methods Eng.*, 7:574–575, 1973.

[4] P. Frey. Chapter 7. the finite element approximation. https://www.ljll.math.upmc.fr/ frey/ma691.html, 2008.

[5] A.J. Hanson. Geometry for n-Dimensional Graphics, 1994.

[6] E T Jaynes. *Probability Theory The Logic Of Science Edition 1*. Cambridge University Press, 2003.

[7] Alfio Quarteroni. *Numerical models for differential problems*. Springer, Milan New York, 2009.

[8] Joel L. Schiff. *The Laplace Transform*. Springer New York, 1999.

[9] F.J. Vermolen and A. Segal. On an integration rule for products of barycentric coordinates over simplexes in rn. *Journal of Computational and Applied Mathematics*, 330:289 – 294, 2018.