Gauss Quadrature in Triangles

*Report 3 on the course "Numerical Analysis".

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Abstract

This report investigates the Gauss quadrature rules in a triangle and tetrahedron. We use symmetry to reduce the number of equations and variables. Finally, we compare the difference between Gauss quadrature in one or higher dimensions. Also, we discuss the vanilla Newton algorithm and Broyden algorithm to solve the nonlinear equations w.r.t. the weights and coordinates of nodes.

CONTENTS

I. Nonlinear System of Equations

A. Newton iteration

Assume $f \in \mathbb{R}^n \to \mathbb{R}^n$, we want to solve $f(x) = 0$. The following recursive relation is adopted to find the roots

$$x^{(k+1)} = x^{(k)} - \nabla f(x^{(k)})^{-1} f(x^{(k)}) \tag{I.1}$$

In computing $\nabla f(x^{(k)})^{-1} f(x^{(k)})$, we can either calculate $\nabla f(x^{(k)})$ and solve the linear equation in each time, or use Broyden algorithm

$$(A^{(0)})^{-1} = \nabla f(x^{(0)})^{-1} \tag{I.2a}$$

$$(A^{(k)})^{-1} - (A^{(k-1)})^{-1} = -\frac{[(A^{(k-1)})^{-1} g^{(k-1)} - y^{(k-1)}](y^{(k-1)})^\top (A^{(k-1)})^{-1}}{(y^{(k-1)})^\top (A^{(k-1)})^{-1} g^{(k-1)}} \tag{I.2b}$$

where

$$g^{(k-1)} = f(x^{(k)}) - f(x^{(k-1)}) \tag{I.3a}$$

$$y^{(k-1)} = x^{(k)} - x^{(k-1)} \tag{I.3b}$$

In our implementation, we use variable “flag” to differentiate these two cases.

B. Homotopy method

We use the homotopy function

$$h(x, \lambda) = f(x) + (\lambda - 1) f(x_0) \tag{I.4}$$

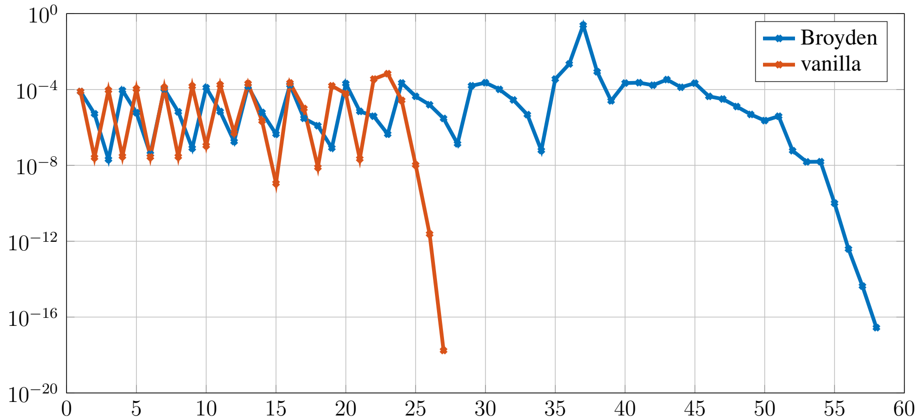
and we take $\lambda_i = \frac{i}{n}$ in the i-th iteration. When $\lambda_i < 1$, we set the stopping rule to be $\|h(x, \lambda_i)\|_\infty < 10^{-6}$. When $\lambda = 1$, the stopping rule is set to be $\|f(x)\|_\infty < 2^{-52}$.

C. Comparison between two cases

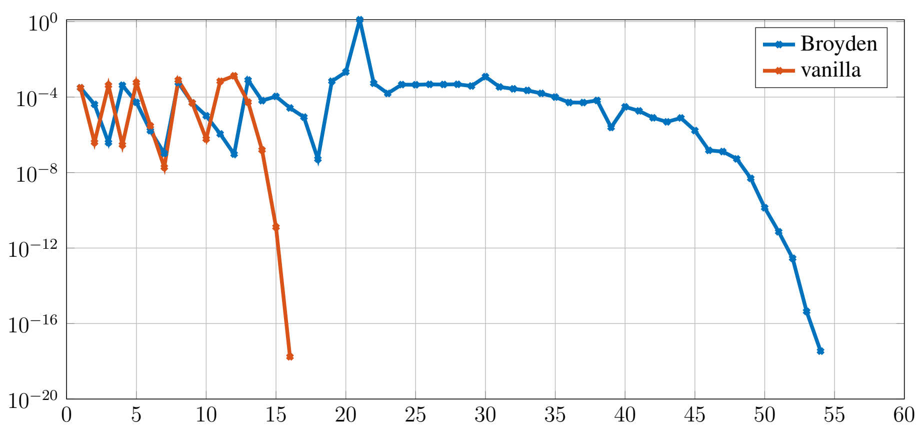
We use the objective function from “test4.m” to compare the performace between these two cases in “test5.m”. We have the following table I.1, we find that vanilla method is more stable than Broyden algorithm.

Then, we explore the trajectory of infinity error, we set the initial point to be $(0, 0, 0, 0)^\top$, and vary the number of homotopy classes. The results are plotted in Figure I.1 and I.2.

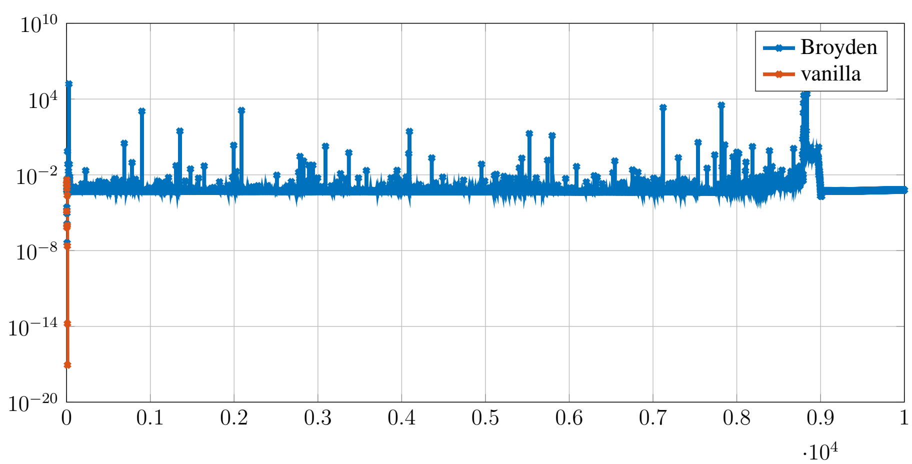
We find that more homotopy classes are crucial for convergence, especially for Broyden algorithm, which fails to converge when the number of classes is 2 but is able to converge when the number of



(a) num of homotopy classes = 10

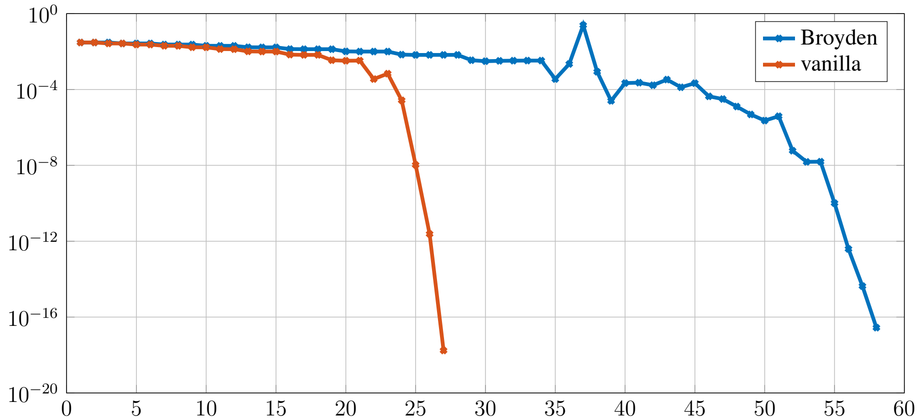


(b) num of homotopy classes = 5

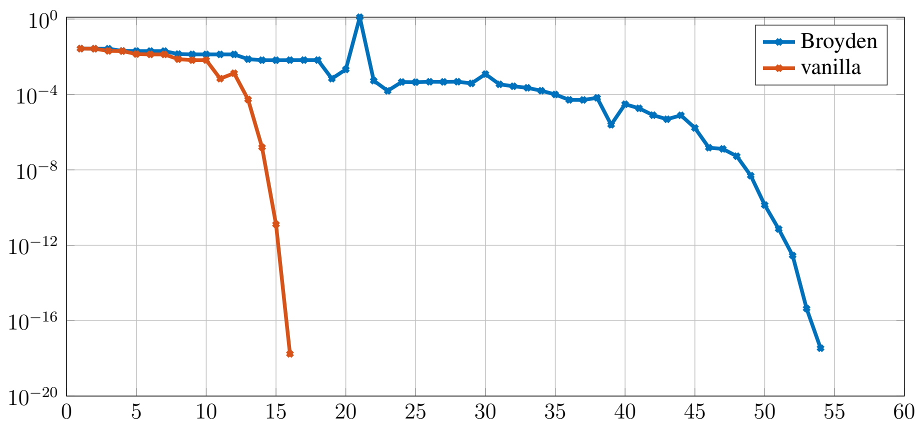


(c) num of homotopy classes= 2

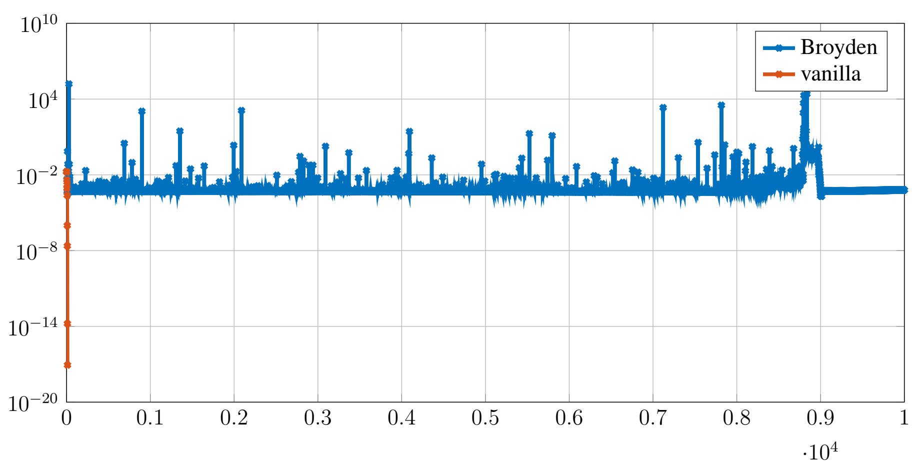
Fig. I.1. ℓ_∞ error of homotopy function $H(x, \lambda)$



(a) num of homotopy classes = 10



(b) num of homotopy classes = 5



(c) num of homotopy classes= 2

Fig. I.2. ℓ_∞ error of objective function $f(x)$

TABLE I.1
COMPARISON BETWEEN TWO METHOD

initial point	ℓ_∞ error		iter		time	
	Broyden	vanilla	Broyden	vanilla	Broyden	vanilla
$(0, 0, 0, 0)^\top$	2.7756e-17	1.7347e-18	58	27	0.0135	0.0067
$(1, 0, 0, 0)^\top$	6.9389e-18	3.4694e-18	301	36	0.0149	0.0087
$(1, 1, 0, 0)^\top$	1.2250e+25	3.4694e-18	max	36	0.0922	0.0068
$(1, 1, 0, 0)^\top$	5.7000e-03	3.4694e-18	max	57	0.0815	0.0073
$(1, 1, 1, 1)^\top$	8.5001e-17	5.2042e-18	168	36	0.0147	0.0061
$(0.5, 0.5, 0.5, 0.5)^\top$	∞	5.2042e-18	max	231	0.0874	0.0171

classes is 5. Generally, vanilla Newton iteration requires fewer iterations than Broyden algorithm, while requires more computational budgets from solving the linear equations.

Then, we compare the Figure I.1 and I.2, we find that solving $H(x, \lambda) = 0$ for $\lambda \neq 1$ only slowly decreases the error of the residual, but is crucial for convergence. The order of convergence in the neighborhood of optimal point is second order.

II. Triangle

We can use a linear transformation to transform any triangle into the standard triangle, whose vertices are $(0, 0), (0, 1), (1, 0)$. Assume the vertices of the original triangle is $(x_i, y_i), 1 \leq i \leq 3$, the linear transformation is

$$\begin{aligned} x(s,t) &= x_1 + (x_2 - x_1)s + (x_3 - x_1)t \\ y(s,t) &= y_1 + (y_2 - y_1)s + (y_3 - y_1)t \end{aligned} \tag{II.1}$$

Hence, $\frac{\partial(x,y)}{\partial(s,t)} = 2Area$, and

$$I(f) = 2Area \int_{s=0}^{1} \int_{t=0}^{1-s} f(x(s,t), y(s,t)) dt ds \tag{II.2}$$

Thus, we need only compute nodes and weights on a standard triangle.

A. Polynomials of order 1

We only use one node.

$$f(s,t) = 1 \quad w_1 = \frac{1}{2} \tag{II.3a}$$

$$f(s,t) = s \quad w_1 x_1 = \frac{1}{6} \tag{II.3b}$$

$$f(s,t) = t \quad w_1 y_1 = \frac{1}{6} \tag{II.3c}$$

To sum up, we have the node is $(\frac{1}{3}, \frac{1}{3})$ and weight is $\frac{1}{2}$. We plot our results in figure II.1.

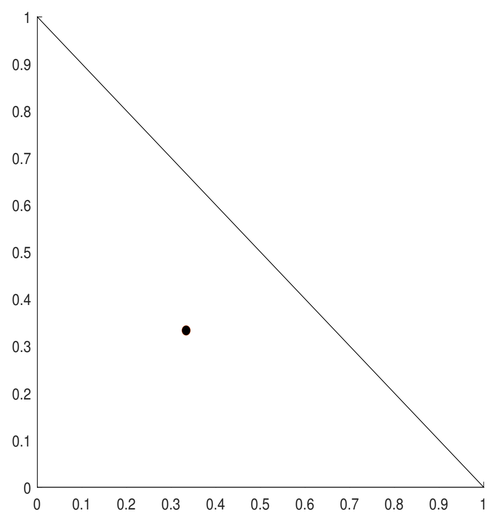


Fig. II.1. Polynomials of order 1

B. Polynomials of order 2

We first shows that two points are not enough. Otherwise,

$$f(s,t) = 1 \quad w_1 + w_2 = \frac{1}{2} \tag{II.4a}$$

$$f(s,t) = s \quad w_1 x_1 + w_2 x_2 = \frac{1}{6} \tag{II.4b}$$

$$f(s,t) = t \quad w_1 y_1 + w_2 y_2 = \frac{1}{6} \tag{II.4c}$$

$$f(s,t) = s^2 \quad w_1 x_1^2 + w_2 x_2^2 = \frac{1}{12} \tag{II.4d}$$

$$f(s,t) = t^2 \quad w_1 y_1^2 + w_2 y_2^2 = \frac{1}{12} \tag{II.4e}$$

$$f(s,t) = st \quad w_1 x_1 y_1 + w_2 x_2 y_2 = \frac{1}{24} \tag{II.4f}$$

We prove that the function have no solution.

- **Proof**:

  Assume the solution exist, then we have

$$\begin{aligned} f(s,t) &= w_1(x_1 s + y_1 t + 1)^2 + w_2(x_2 s + y_2 t + 1)^2 \\ &= \frac{1}{12}(s^2 + t^2 + st) + \frac{1}{3}(s+t) + \frac{1}{2} \\ &= \frac{1}{12}((s + \frac{t}{2} + 2)^2 + \frac{3}{4}(t + \frac{4}{3})^2 + \frac{2}{3}) > 0 \end{aligned} \tag{II.5}$$

  Besides, we $x_1 y_2 \neq x_2 y_1$, otherwise,

$$(w_1 x_1^2 + w_2 x_2^2)(w_1 y_1^2 + w_2 y_2^2) = (w_1 x_1 y_1 + w_2 x_2 y_2)^2$$

  which is contrary to equations II.4. Thus, there exist s, t, such that

$$x_1 s + y_1 t + 1 = x_2 s + y_2 t + 1 = 0$$

  which leads to $f(s,t) = 0$, contrary to the fact that $f(s,t) > 0$. In sequel, the set of equations has no real roots. There are at least three node points.

Then, when there are three points, we have

$$f(s,t) = 1 \quad w_1 + w_2 + w_3 = \frac{1}{2} \tag{II.6a}$$

$$f(s,t) = s \quad w_1 x_1 + w_2 x_2 + w_3 x_3 = \frac{1}{6} \tag{II.6b}$$

$$f(s,t) = t \quad w_1 y_1 + w_2 y_2 + w_3 y_3 = \frac{1}{6} \tag{II.6c}$$

$$f(s,t) = s^2 \quad w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2 = \frac{1}{12} \tag{II.6d}$$

$$f(s,t) = t^2 \quad w_1 y_1^2 + w_2 y_2^2 + w_3 y_3^2 = \frac{1}{12} \tag{II.6e}$$

$$f(s,t) = st \quad w_1 x_1 y_1 + w_2 x_2 y_2 + w_3 x_3 y_3 = \frac{1}{24} \tag{II.6f}$$

Assuming $x_1 = 0, y_2 = 0, x_3 + y_3 = 1$, we have

$$w_1 + w_2 + w_3 = \frac{1}{2} \tag{II.7a}$$
$$w_2 x_2 + w_3 x_3 = \frac{1}{6} \tag{II.7b}$$
$$w_1 y_1 + w_3(1 - x_3) = \frac{1}{6} \tag{II.7c}$$
$$w_2 x_2^2 + w_3 x_3^2 = \frac{1}{12} \tag{II.7d}$$
$$w_1 y_1^2 + w_2 y_2^2 + w_3 y_3^2 = \frac{1}{12} \tag{II.7e}$$
$$w_3 x_3(1 - x_3) = \frac{1}{24} \tag{II.7f}$$

The solution can clearly be obtained by $w_i = \frac{1}{6}, t = \frac{1}{2}$. The code is implmented in "test1.m", where we take initial value $x^{(0)} = x^\star + \varepsilon N(0, I)$, $x^\star = (\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

Another approach, which is more inspiring, is by symmetry. Clearly, we should anticipate that $w_1 = w_2 = w_3 := w$, and

$$\begin{aligned}(x_2, y_2) &= (1, 0) + y_1(-1, 0) + x_1(-1, 1)\\ (x_3, y_3) &= (0, 1) + y_1(1, -1) + x_1(0, -1)\end{aligned} \tag{II.8}$$

Clearly, from equation II.6a, $w = \frac{1}{6}$. Hennce, only two variables remains. Equation II.6b, II.6c hold, and equation II.6d, II.6e, II.6f are equivalent. Hence, we have

$$x_1^2 + (1 - x_1 - y_1)^2 + y_1^2 = \frac{1}{2} \tag{II.9}$$

which constitutes an ellipse inscribes the triangle.

Codes to generate the figure II.2:

```
patch([0,1,0],[0,0,1],[1,1,1])
fimplicit(@(x,y) x.^2+y.^2+(1-x-y).^2-1/2)
scatter(0.0931,0.2533,'fill','k')
scatter(1-0.0931-0.2533,0.0931,'fill','k')
scatter(0.2533,1-0.0931-0.2533,'fill','k')
```

Hence, there are infinite nodes choices, $(s, t), (1-s-t, s), (t, 1-s-t)$, where $s^2+t^2+(1-s-t)^2 = \frac{1}{2}$, and unified weights $w_i = \frac{1}{6}$.

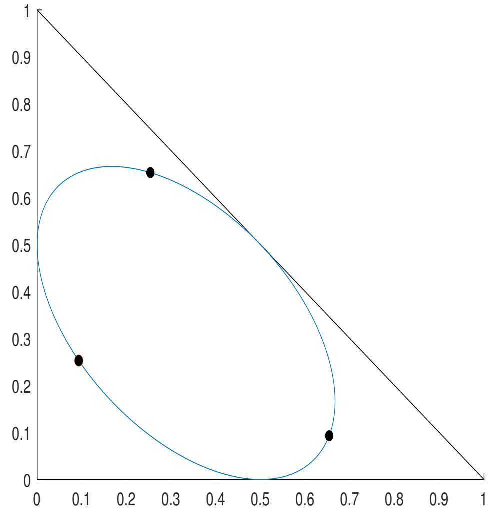


Fig. II.2. Polynomials of order 2

C. Polynomials of order 3

Since there are 10 equations, i.e. $1, x, y, x^2, xy, y^2, x^3, x^2y,$ xy^2, y^3 in total, at least 4 node points are required, leading to 12 variables. By symmetry, we can assume one of the node is $(\frac{1}{3}, \frac{1}{3})$ with weight w_2, and the other three node points are in the form $(s,t), (1-s-t, s), (t, 1-s-t)$, with unified weight w_1. We thus have $3w_1 + w_2 = \frac{1}{2}$ by setting $f(x,y) = 1$ or x.

Hence, we have

$$3w_1 + w_2 = \frac{1}{2} \tag{II.10a}$$

$$w_1(s^2 + t^2 + (1-s-t)^2) + w_2\frac{1}{9} = \frac{1}{12} \tag{II.10b}$$

$$w_1(s^2t + (1-s-t)^2s + s^2(1-s-t)) + w_2\frac{1}{9} = \frac{1}{60} \tag{II.10c}$$

$$w_2(s^3 + t^3 + (1-s-t)^3) + w_2\frac{1}{27} = \frac{1}{20} \tag{II.10d}$$

Another criterion

$$w_1(st + (1-s-t)(s+t)) + w_2\frac{1}{9} = \frac{1}{24} \tag{II.11}$$

is equivalent to II.10a and II.10b.

We use “test2.m” to compute the solution of II.10. The initial point is set to be $\mathbf{x}^{(0)} = (0,0,0) + \varepsilon N(0, I)$. The obtained solution is

$$s = t = 1/5, w_2 = -\frac{9}{32} \tag{II.12}$$

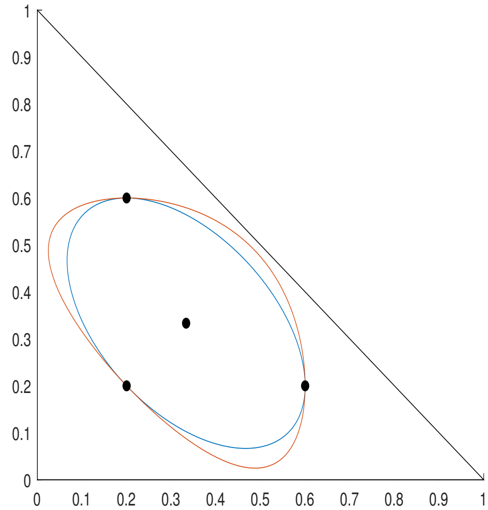


Fig. II.3. Polynomials of order 3

From other initial points, we are able to obtain other solutions. However, they are either equivalent to the solution II.12 or outside the reference triangle, which is not preferrable.

D. Results on a equilateral triangle

a) Polynomials of order 1: The node is $\left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right)$, and the weight is $\frac{\sqrt{3}}{4}$.

b) Polynomials of order 2: The nodes are on the circle $C = \{\left(x - \frac{1}{2}\right)^2 + \left(y - \frac{\sqrt{3}}{6}\right)^2 = \frac{1}{12}\}$, being the vertices of the inscribed equilateral triangle of the circle C, with weight $\frac{\sqrt{3}}{12}$.

c) Polynomials of order 3: The nodes are $\left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right)$ with weight $-\frac{27\sqrt{3}}{192}$, $\left(\frac{3}{10}, \frac{\sqrt{3}}{10}\right)$, $\left(\frac{7}{10}, \frac{\sqrt{3}}{10}\right)$, $\left(\frac{1}{2}, \frac{3\sqrt{3}}{10}\right)$ with weight $\frac{25\sqrt{3}}{192}$.

III. Tetrahedron

We can use a linear transformation to transform any tetrahedron into the standard one, whose vertices are $(0,0,0), (1,0,0), (0,1,0), (0,0,1)$. Assume the vertices of the original triangle is $(x_i, y_i, z_i), 1 \leq i \leq 4$, the linear transformation is

$$\begin{aligned} x(u,v,w) &= x_1 + (x_2 - x_1)u + (x_3 - x_1)v + (x_4 - x_1)w \\ y(u,v,w) &= y_1 + (y_2 - y_1)u + (y_3 - y_1)v + (y_4 - y_1)w \\ z(u,v,w) &= z_1 + (z_2 - z_1)u + (z_3 - z_1)v + (z_4 - z_1)w \end{aligned} \tag{III.1}$$

Hence, $\frac{\partial(x,y,z)}{\partial(u,v,w)} = 6Volume$, and

$$I(f) = 6\text{Volume} \int_{u=0}^{1} \int_{v=0}^{1-u} \int_{w=0}^{1-u-v} f(x(u,v,w), y(u,v,w), z(u,v,w))dudvdw \tag{III.2}$$

Thus, we need only compute nodes and weights on a standard tetrahedron, then the nodes can be transformed according to III.1, and the weights w can be transformed to $6\text{Volume} \times w$. We plot the standard tetrahedron in the following code

```
h = patch('Vertices',[0 0 0; 1 0 0;
 0 1 0; 0 0 1],'Faces',[1 3 2;1 2 4;
 1 3 4;2 3 4],'FaceColor',[1 1 1])
view(3)
alpha(0)
```

A. Polynomials of order 1

Setting $f = 1$, we have $w_1 = \frac{1}{6}$. Besides, setting $f(x,y,z) = x$, we have $w_1 x_1 = \frac{1}{24}$, then $x = \frac{1}{4}$. By symmetry, the node is $\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$.

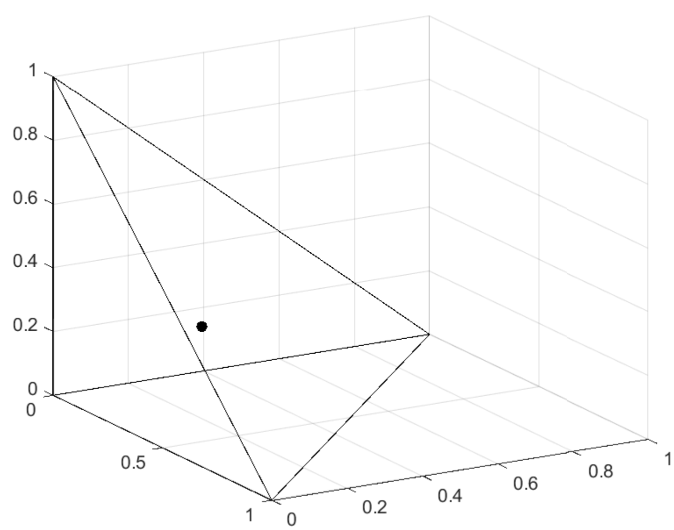


Fig. III.1. Polynomials of order 1, 3 dimension

B. Polynomials of order 2

Since there are $x^2, y^2, z^2, xy, yz, xz, x, y, z, 1$ (10 constraints), and each node provides us with 4 variables, we need at least three nodes. By symmetry, we need four nodes for symmetry. Since the weights are the same, we have the unified weight to be $w = \frac{1}{24}$. The nodes should be

$$\mathbf{x}_1 = (x, y, z)^\top, \mathbf{x}_2 = (1-x-y-z, x, y)^\top, \mathbf{x}_3 = (z, 1-x-y-z, x)^\top, \mathbf{x}_4 = (y, z, 1-x-y-z)^\top \quad \text{(III.3)}$$

We have the following equation

$$x^2 + y^2 + z^2 + (1-x-y-z)^2 = \frac{2}{5} \quad \text{(III.4a)}$$

$$(1-x-z)(x+z) = \frac{1}{5} \quad \text{(III.4b)}$$

$$(1-y-z)(x+y) = \frac{1}{5} \quad \text{(III.4c)}$$

$$(1-x-y)(x+y) = \frac{1}{5} \quad \text{(III.4d)}$$

Note that adding the last three equations up, we get the first equation. We solve this equation in "test3.m". Clearly, the solution has multiple solutions. The results is

$$\begin{aligned} \mathbf{x}_1 &= (0.5854, 0.1382, 0.1382)^\top, \mathbf{x}_2 = (0.1382, 0.5854, 0.1382)^\top \\ \mathbf{x}_3 &= (0.1382, 0.1382, 0.5854)^\top, \mathbf{x}_4 = (0.1382, 0.1382, 0.1382)^\top \end{aligned} \quad \text{(III.5)}$$

if we restrict the nodes to be inside the tetrahedron. The exact solution is $x = y = z = \frac{5-\sqrt{5}}{10}$.

The program produces other results,

$$\begin{aligned} \mathbf{x}_1 &= (0.3618, 0.3618, 0.3618)^\top, \mathbf{x}_2 = (-0.0854, 0.3618, 0.3618)^\top \\ \mathbf{x}_3 &= (0.3618, -0.0854, 0.3618)^\top, \mathbf{x}_4 = (0.3618, 0.3618, -0.0854)^\top \end{aligned} \quad \text{(III.6)}$$

which is outside the tetrahedron.

C. Polynomials of order 3

If there are only 4 points, we have

$$(0.1382^3 + 0.1382^3 + 0.1382^3 + 0.5854^3)/24 \neq \frac{1}{120} = \int_\Delta x^3 \mathrm{d}V$$

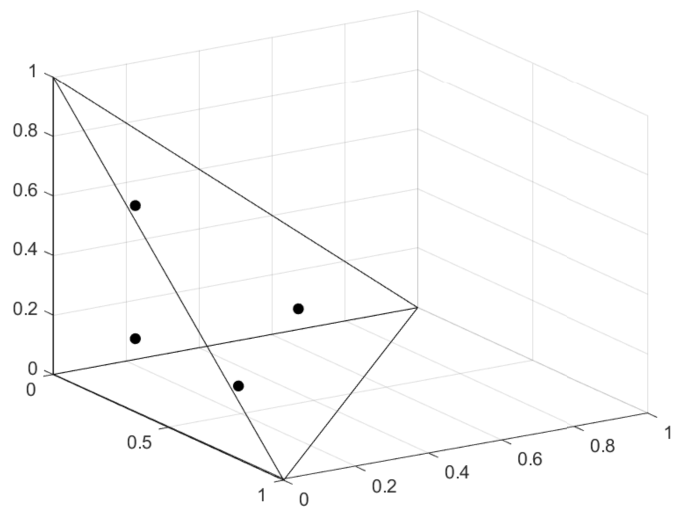


Fig. III.2. Polynomials of order 2, 3 dimension

which means 4 points are not enough. Hence, at least 5 points are required. Still, by symmetry, we assume one of the points is $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})^\top$ with weight w_2 and the other three points

$$\mathbf{x}_1 = (x, y, z)^\top, \mathbf{x}_2 = (1-x-y-z, x, y)^\top, \mathbf{x}_3 = (z, 1-x-y-z, x)^\top, \mathbf{x}_4 = (y, z, 1-x-y-z)^\top \quad \text{(III.7)}$$

with weight w_1. Hence, by setting the degree of function to be zero or one, we have

$$4w_1 + w_2 = \frac{1}{6} \quad \text{(III.8)}$$

Besides, by setting the degree of function to be 2.

$$w_1(x^2 + y^2 + z^2 + (1-x-y-z)^2) + w_2\frac{1}{16} = \frac{1}{60} \quad \text{(III.9a)}$$
$$w_1(1-x-z)(x+z) + w_2\frac{1}{16} = \frac{1}{120} \quad \text{(III.9b)}$$
$$w_1(1-y-z)(x+y) + w_2\frac{1}{16} = \frac{1}{120} \quad \text{(III.9c)}$$
$$w_1(1-x-y)(x+y) + w_2\frac{1}{16} = \frac{1}{120} \quad \text{(III.9d)}$$

Since III.9a can be derived from other equations, we use the following set of equations to obtain the results

$$
\begin{aligned}
4w_1 + w_2 &= \frac{1}{6} && \text{(III.10a)}\\
w_1(1-x-z)(x+z) + w_2\frac{1}{16} &= \frac{1}{120} && \text{(III.10b)}\\
w_1(1-y-z)(x+y) + w_2\frac{1}{16} &= \frac{1}{120} && \text{(III.10c)}\\
w_1(1-x-y)(x+y) + w_2\frac{1}{16} &= \frac{1}{120} && \text{(III.10d)}\\
w_1(x^3+y^3+z^3+(1-x-y-z)^3)1 + w_2\frac{1}{64} &= \frac{1}{120} && \text{(III.10e)}
\end{aligned}
$$

which is implmented in "test4.m". The results are

$$
w_1 = \frac{3}{40}, w_2 = -\frac{2}{15}, \quad x = y = z = \frac{1}{6} \tag{III.11}
$$

To validate the solution indeed satisfies all polynomials whose degree is not larger than 3. We still need to verify (by symmetry, if $f(x,y,z) = x^2y$ is satisfied, then $f(x,y,z) = y^2x, y^2z, z^2y, x^2z, z^2x$ are also satisfied.)

$$
\begin{aligned}
w_1(x^2y + (1-x-y-z)^2x + z^2(1-x-y-z) + y^2z) + w_2\frac{1}{64} &= \int_\Delta x^2y\mathrm{d}V\\
w_1(xyz + (xy+yz+zx)(1-x-y-z)) + w_2\frac{1}{64} &= \int_\Delta xyz\mathrm{d}V
\end{aligned} \tag{III.12}
$$

which are correct by direct computation

$$
\int_\Delta x^2y\mathrm{d}V = \int_0^1 x^2dx\int_0^{1-x} ydy\int_0^{1-x-y} dz = \int_0^1 x^2dx\int_0^{1-x}(1-x-y)ydy = \frac{1}{360}
$$

and

$$
\begin{aligned}
\int_\Delta xyz\mathrm{d}V = \int_0^1 xdx\int_0^{1-x} ydy\int_0^{1-x-y} zdz &= \int_0^1 xdx\int_0^{1-x}\frac{1}{2}y(1-x-y)^2dy\\
&= \frac{1}{24}\int_0^1 x(1-x)^4dx = \frac{1}{720}
\end{aligned}
$$

IV. Summary

A. Summary of codes

- **newton_homotopy**: implements the Newton's method to solve nonlinear equations with homotopy method.
- **test1**: Find nodes and weights in a triangle second order algebraic precision.

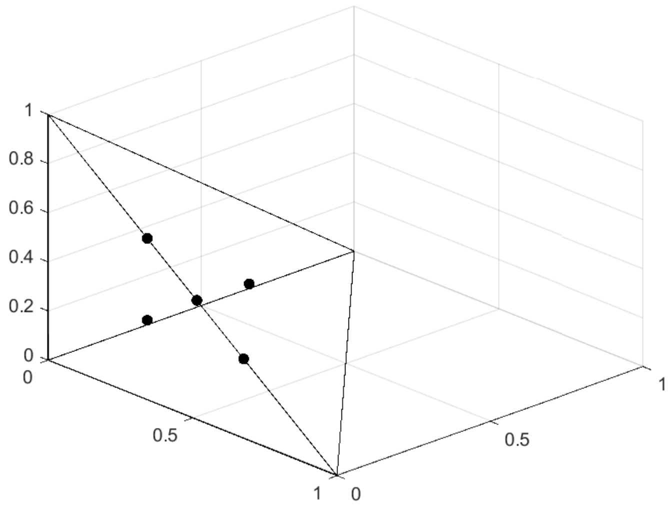


Fig. III.3. Polynomials of order 3, 3 dimension

- **test2**: Find nodes and weights in a triangle third order algebraic precision.
- **test3**: Find nodes and weights in a tetrahedron second order algebraic precision.
- **test4**: Find nodes and weights in a tetrahedron second order algebraic precision.
- **test5**: Comparison between vanilla Newton's iteration (flag = 0) as well as Broyden algorithm (flag = 1).

B. Summary of experiments

In all our experiments, the validity of solution is obtained by calculating the residual of the solution and verified by the fact that the scale of the residual is below the machine epsilon (2^{-52}). We have the following two observation.

1) The nodes and corresponding weights might not be unique given a reference region.
2) The nodes could be outside the region and the weights could be negative.

which are completely different from one-dimensional Gauss quadrature rule, where nodes are uniquely inside the region and weights are guaranteed to be positive.