Numerical integration in more dimensions – part 2

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Outline

The role of a mapping function in multidimensional integration

Gauss approach in more dimensions and quadrature rules

Critical analysis of acceptability of a given quadrature rule
Problem definition

- We have \( f : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R} \) and we want to compute \( I \):

  \[
  I = \int_\Omega f \, dx
  \]

- We want to implement some numerical method, which ought to be (as usual) **accurate** and **cheap** (e.g. small number of operations)
Covering

Step 1: covering of the domain with replicas of a basic geometry

\[ \int_{\Omega} f(x)dx \approx \sum_{1}^{n} \int_{e_1} f(x)dx \]

Error 1: covering error
Mapping function

- Step 2: introduction of a mapping function $F$
  - Example 1: squares

$$F_1 \left( \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right) = \left[ \begin{array}{c} v_{1}^{(1)} - v_{0}^{(1)} \\ v_{2}^{(1)} - v_{0}^{(1)} \end{array} \right] \left[ \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right] + v_{0}^{(1)}$$

$$= A_1 \hat{x} + b_1$$
Mapping function

- example 2: triangles

\[
F_1 \left( \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right) = \left[ \begin{array}{c} v_1^{(1)} - v_0^{(1)} \\ v_2^{(1)} - v_0^{(1)} \end{array} \right] \left[ \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right] + v_0^{(1)}
= A_1 \hat{x} + b_1
\]
Properties of the mapping function $F$

- $F_1$ is affine: $F_1(\hat{\mathbf{x}}) = A_1 \hat{\mathbf{x}} + \mathbf{b}_1$

$F$ maps affine combinations

$$\sum_i \alpha_i x_i, \quad \sum_i \alpha_i = 1$$

to affine combinations

…that is, triangles are mapped to triangles, rectangles to parallelograms, etc.
The role of the mapping function

- **Step 1:** \[ \int_{\Omega} f(x) \, dx \equiv \sum_{i} \int_{e_i} f(x) \, dx \]

- **Step 2:**
  \[ \int_{e_1} f(x) \, dx = \int f(F_1(\hat{x})) \left| det(\partial F_1) \right| d\hat{x} = \]
  \[ = \left| det(A_1) \right| \int f(F_1(\hat{x})) d\hat{x} \]
Step 3: integration over the basic geometry

\[ \int_{\hat{e}} f(\hat{F}(\hat{x})) d\hat{x} = \int_{\hat{e}} g(\hat{x}) d\hat{x} \approx \sum_{i} w_i g(\hat{x}_i) \]

Error 2: quadrature error
Integration over a surface

- Suppose we have a function defined over a surface
- Thanks to the properties of the mapping function, we can use the same approach:

\[
F_1 \left( \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right) = \left[ \begin{array}{c} v_1^{(1)} - v_0^{(1)} \\ v_2^{(1)} - v_0^{(1)} \end{array} \right] \left[ \begin{array}{c} \hat{x} \\ \hat{y} \end{array} \right] + v_0^{(1)} = A_1 \hat{x} + b_1
\]

...simply \( v^{(1)} \) given in a suitable reference system...
How can one reduce errors?

**Covering error**

**Quadrature error**

- More accurate formulas
- Smaller volumes (where necessary, depending on f)
Open problem

Given a basic geometry, find the least amount of points and weights such that

\[ \int g(\hat{x})d\hat{x} \approx \sum_i w_i g(\hat{x}) \]

is exact for all monomials of degree \( d \) and lower

- Let’s look at some examples…
d=1 in the square

3 equations $\Rightarrow$ 1 point, 1 weight

Mathematical problem - Physical interpretation

\[
\begin{align*}
\int_{\hat{\mathbf{e}}} 1 \, dx \, dy &= 1 = w_1 \\
\int_{\hat{\mathbf{e}}} x \, dx \, dy &= \frac{1}{2} = w_1 \hat{x}_1 \\
\int_{\hat{\mathbf{e}}} y \, dx \, dy &= \frac{1}{2} = w_1 \hat{y}_1
\end{align*}
\]
d=1 in the triangle

3 equations $\rightarrow$ 1 point, 1 weight

Mathematical problem - Physical interpretation

\[
\begin{align*}
\int_{\hat{e}} 1 \, dx \, dy &= \frac{1}{2} = w_1 \\
\int_{\hat{e}} x \, dx \, dy &= \frac{1}{6} = w_1 \hat{x}_1 \\
\int_{\hat{e}} y \, dx \, dy &= \frac{1}{6} = w_1 \hat{y}_1
\end{align*}
\]

$\hat{w}_1 = \frac{1}{2}$
d=2 in the square

6 equations → 2 points, 2 weights

Mathematical problem - Physical interpretation

\[ \int_0^1 dx \int_0^1 dy = 1 = w_1 + w_2 \]
\[ \int_0^1 dx \int_0^1 dy = \frac{1}{2} = w_1 \hat{x}_1 + w_2 \hat{x}_2 \]
\[ \int_0^1 dx \int_0^1 dy = \frac{1}{2} = w_1 \hat{y}_1 + w_2 \hat{y}_2 \]
\[ \int_0^1 dx \int_0^1 dy = \frac{1}{3} = w_1 \hat{x}_1^2 + w_2 \hat{x}_2^2 \]
\[ \int_0^1 dx \int_0^1 dy = \frac{1}{3} = w_1 \hat{y}_1^2 + w_2 \hat{y}_2^2 \]
\[ \int_0^1 dx \int_0^1 dy = \frac{1}{4} = w_1 \hat{x}_1 \hat{y}_1 + w_2 \hat{x}_2 \hat{y}_2 \]

...no Mathematica solution...

16/10/2002 Seminar: Numerical Integration in more dimensions
### d=3 (e.g. in the triangle)

<table>
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<tr>
<th>Equations</th>
<th>Points</th>
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<tr>
<td>10</td>
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</tr>
<tr>
<td>3</td>
<td>too many</td>
</tr>
<tr>
<td>4</td>
<td>not enough</td>
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\[
x - y  \\
x^2 - xy - y^2  \\
x^3 - x^2y - xy^2 - y^3
\]
Let’s choose two monomials $p(x)$ and $q(y)$ and let them be of degree $d$ at most.

If we choose $d=3$.

16 equations $\rightarrow$ 4 points, 4 weights

...no Mathematica solution (in a reasonable time)
Cross product Gauss

Gauss 1D in [0,1]

Gauss 2D in [0,1]^2

- only for domains like [a,b]^n

\[ \iint g(x, y) \, dx \, dy = \int \sum_i w_i g(\hat{x}_i, y) \, dy = \sum_i w_i \int g(\hat{x}_i, y) \, dy = \sum_i \sum_j w_i w_j g(\hat{x}_i, \hat{x}_j) \]
Higher degree formulas

- Many of them in the literature

  - Example 1:
    degree 6 in the triangle with 12 points

  - Example 2:
    degree 20 in the triangle with 79 points!


A.H. Stroud & D. Secrest, GAUSSIAN QUADRATURE FORMULA, Prentice-Hall, 1966
Summary

Do the number of the unknowns correspond to the number of the equations?

Does the non-linear system have a solution?

Is the found solution acceptable?

Condition 1: Are all the points $\hat{x}_i$ inside the element?
Condition 2: Are all the weights $w_i$ positive?

WE HAVE AN ACCEPTABLE QUADRATURE METHOD!
Condition 1: \( \hat{X}_i \in \hat{e} \ \forall i \)

What is the value of \( f(F(\hat{x}_4)) \) if \( F(\hat{x}_4) \) does not belong to \( \Omega \)?
Condition 2: $w_i \geq 0, \forall i$

- To always have non-negative integrals for non-negative functions

Exact solution: $\int_a^b f(x) \, dx > 0$

Approximation: $\sum_{i=1}^{7} w_i f(x_i) < 0$ if $w_2 < 0$

- Finite Elements Methods (FEM)
Why weights always $\geq 0$ in FEM

- Stiffness matrix $A$ is positive definite

$$u^T Au = \sum_i \sum_j u_i a_{ij} u_j = \ldots = \int |\nabla u|^2 + u^2 > 0 \quad \text{if } u > 0$$

- Positive definite property is needed for the iterative solvers of Krylov type (all fast iterative solvers)

- Negative weights might cause positive definite property to be lost
Do we really get negative weights?

- Newton-Cotes approach in \([-1,1]\):

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</table>

- Negative weights also in many formula using with Gauss approach
Covering

- Example 2: triangles → more flexible