Numerical integration in more dimensions – part 2

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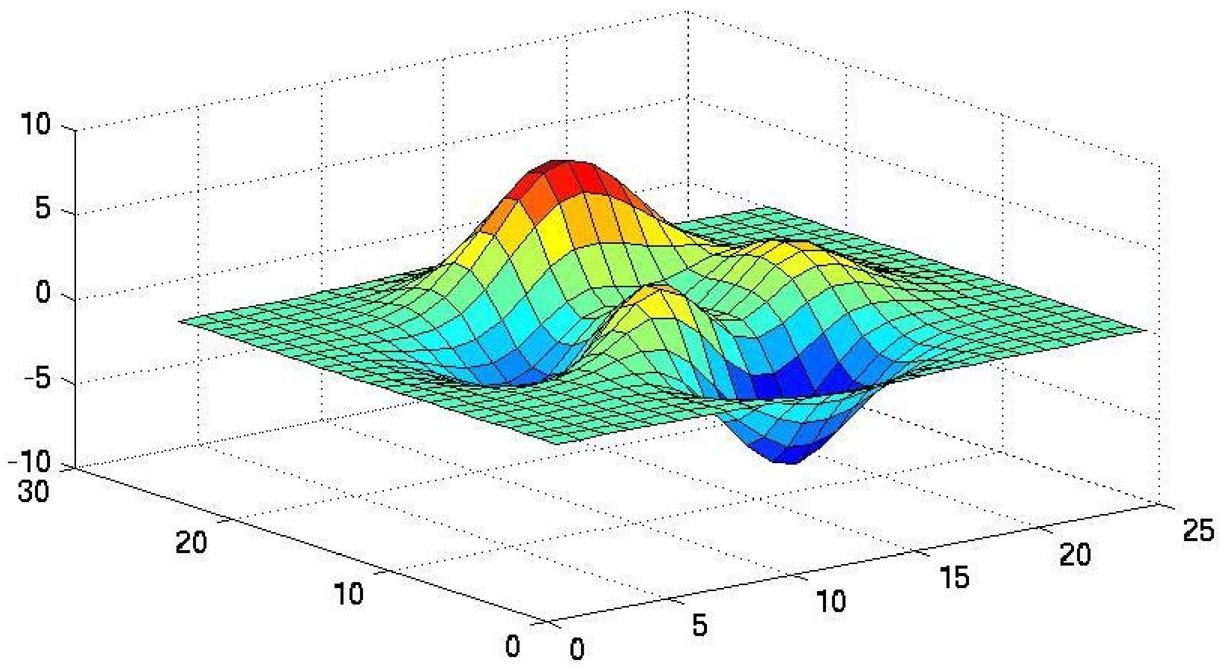


Outline

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 $f : \Omega \subset \Re^n \rightarrow \Re$ and we want to compute I:

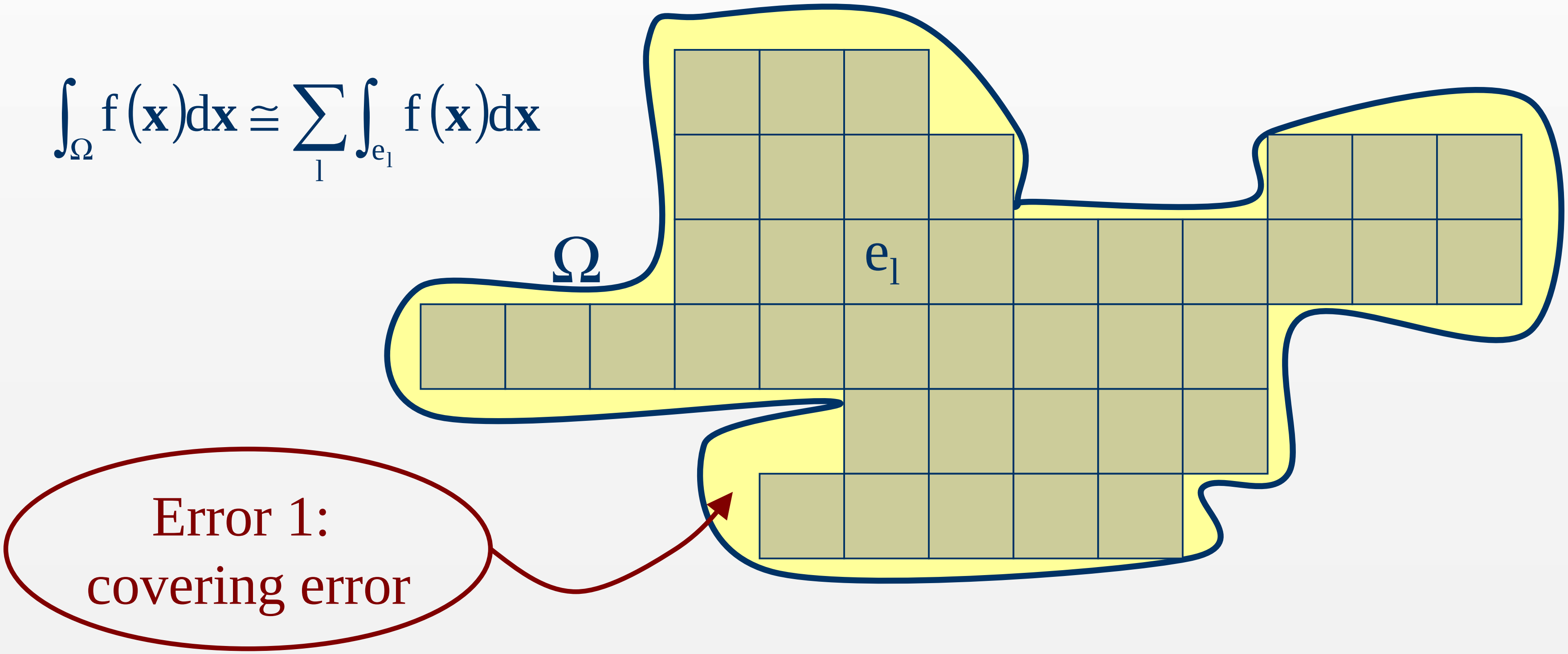
$$I = \int_\Omega f \, d\mathbf{x}$$

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

Covering

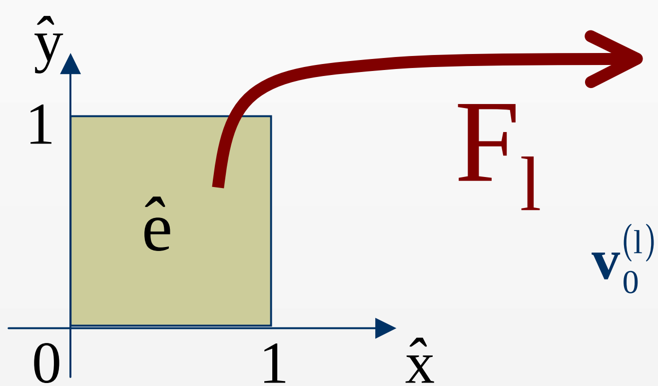
- Step 1: covering of the domain with replicas of a basic geometry

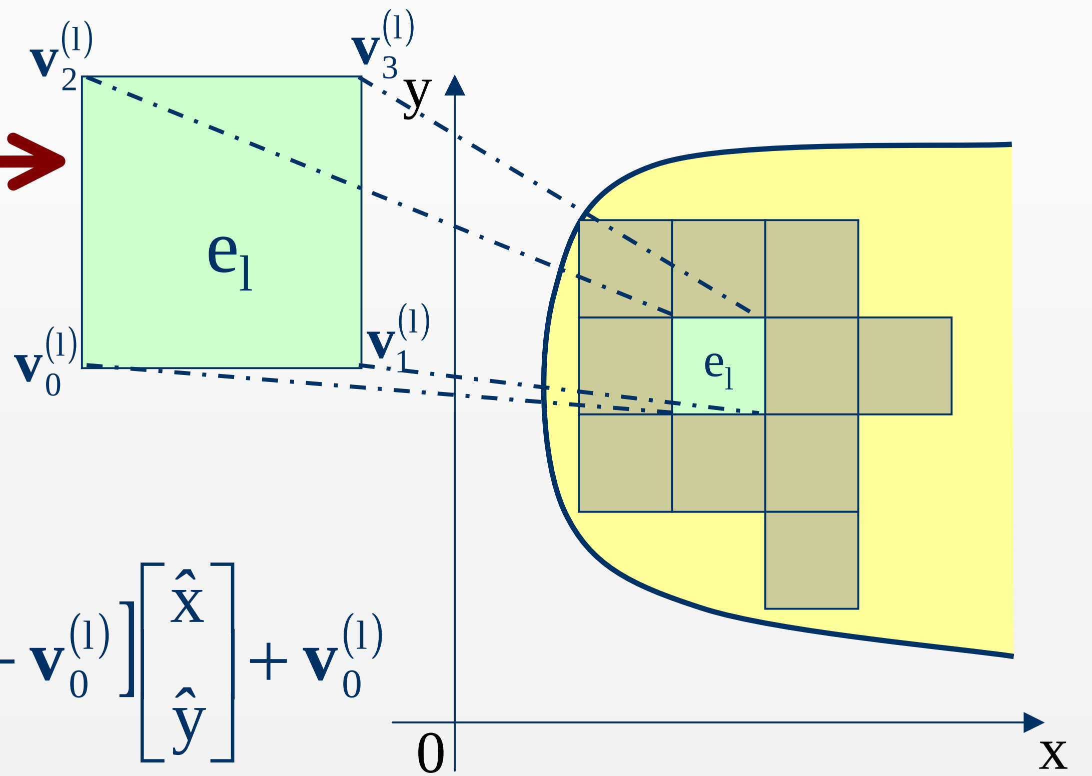
$$\int_{\Omega} f(\mathbf{x})d\mathbf{x} \cong \sum_{l} \int_{e_l} f(\mathbf{x})d\mathbf{x}$$



Mapping function

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



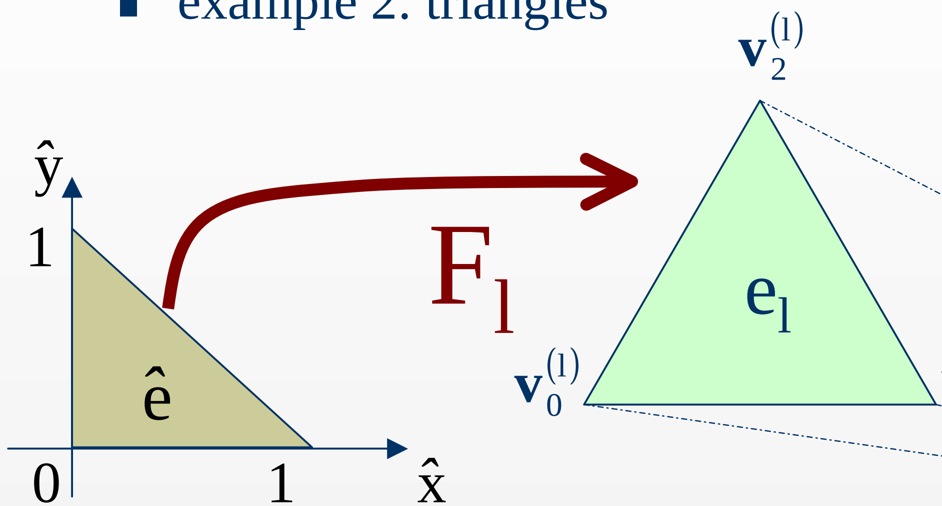


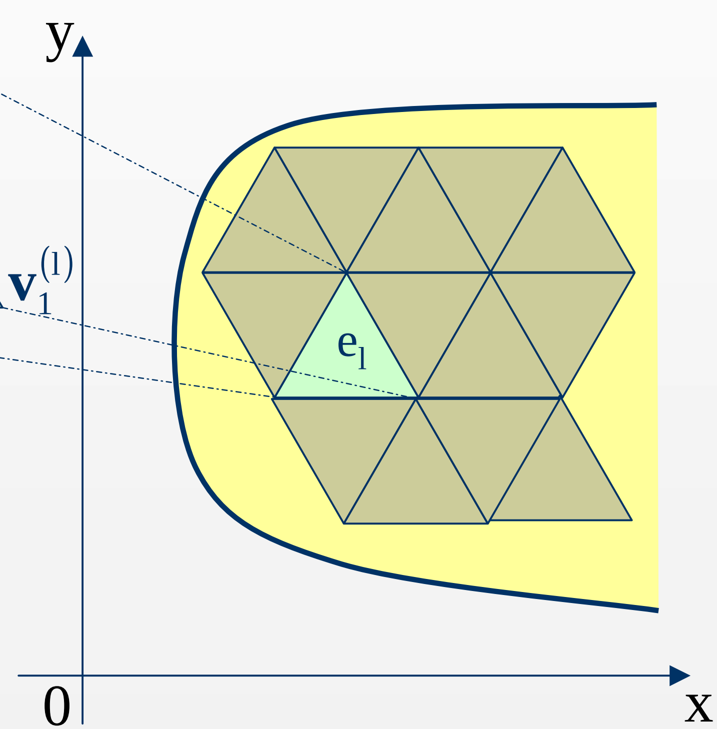
$$F_l\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} = \left[\mathbf{v}_1^{(l)} - \mathbf{v}_0^{(l)} \mid \mathbf{v}_2^{(l)} - \mathbf{v}_0^{(l)}\right]\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix} + \mathbf{v}_0^{(l)}$$

$$= A_l\hat{\mathbf{x}} + \mathbf{b}_l$$

Mapping function

- example 2: triangles





$$F_l\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} = \left[\mathbf{v}_1^{(l)} - \mathbf{v}_0^{(l)} \mid \mathbf{v}_2^{(l)} - \mathbf{v}_0^{(l)}\right]\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix} + \mathbf{v}_0^{(l)}$$

$$= A_l\hat{\mathbf{x}} + \mathbf{b}_l$$

Properties of the mapping function F

- F_l is affine: $F_l(\hat{\mathbf{x}}) = A_l\hat{\mathbf{x}} + \mathbf{b}_l$

  constant

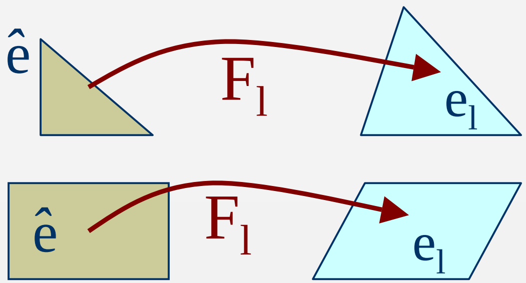
  linear

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: $\int_{\Omega} f(\mathbf{x})d\mathbf{x} \cong \sum_{l} \int_{e_l} f(\mathbf{x})d\mathbf{x}$

- Step 2: $\int_{e_l} f(\mathbf{x})d\mathbf{x} = \int_{\hat{e}} f\left(F_l(\hat{\mathbf{x}})\right)\left|det\left(\partial F_l\right)\right| d\hat{\mathbf{x}} =$

$$= \left|det\left(A_l\right)\right| \cdot \int_{\hat{e}} f\left(F_l(\hat{\mathbf{x}})\right)d\hat{\mathbf{x}}$$

Quadrature

- Step 3: integration over the basic geometry

$$\int_{\hat{e}} f\left(F_l\left(\hat{\mathbf{x}}\right)\right) d\hat{\mathbf{x}} = \int_{\hat{e}} g\left(\hat{\mathbf{x}}\right) d\hat{\mathbf{x}} \cong \sum_i w_i g\left(\hat{\mathbf{x}}_i\right)$$

Error 2:
quadrature error

Integration over a surface

- Suppose we have a function defined over a surface

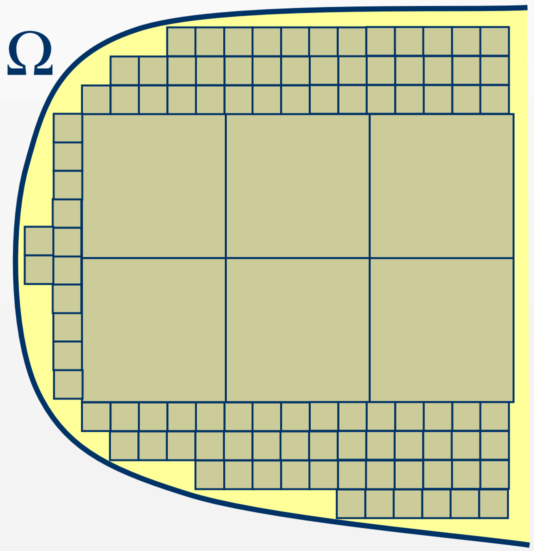
- Thanks to the properties of the mapping function, we can use the same approach:

$$F_l\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} = \left[\mathbf{v}_1^{(l)} - \mathbf{v}_0^{(l)} \mid \mathbf{v}_2^{(l)} - \mathbf{v}_0^{(l)}\right]\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix} + \mathbf{v}_0^{(l)} = A_l\hat{\mathbf{x}} + \mathbf{b}_l$$

…simply $\mathbf{v}^{(l)}$ given in a suitable reference system…

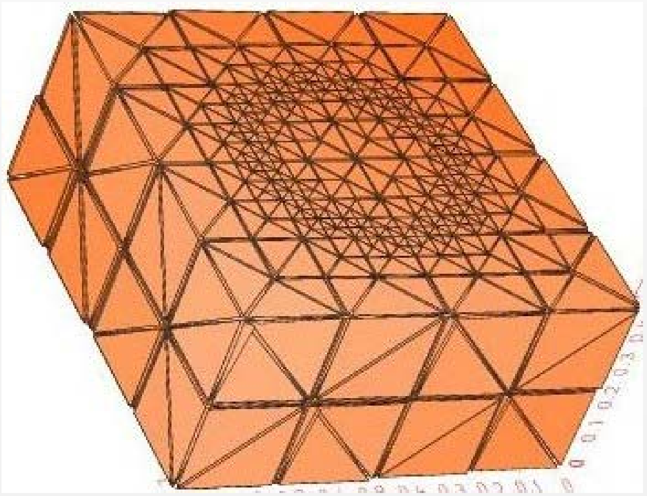
How can one reduce errors?

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

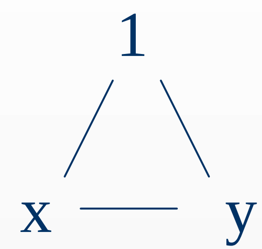
$$\int_{\hat{e}} g(\hat{\mathbf{x}})d\hat{\mathbf{x}} \cong \sum_{i} w_i g(\hat{\mathbf{x}})$$

is exact for all monomials of degree d and lower

- Let’s look at some examples…

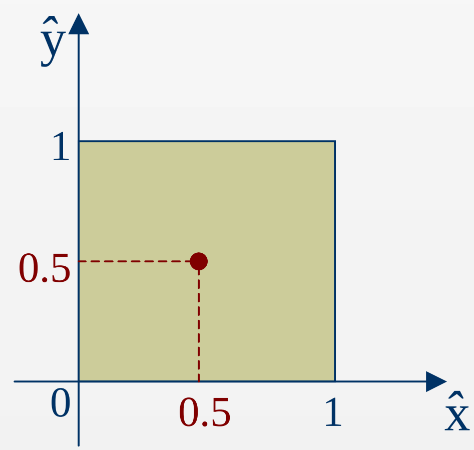
d=1 in the square

3 equations → 1 point, 1 weight



Mathematical problem - Physical interpretation

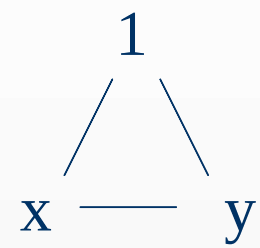
$$
\begin{cases}
\int_{\hat{e}} 1 \, dx \, dy = 1 = w_1 \\
\int_{\hat{e}} x \, dx \, dy = \frac{1}{2} = w_1 \hat{x}_1 \\
\int_{\hat{e}} y \, dx \, dy = \frac{1}{2} = w_1 \hat{y}_1
\end{cases}
$$



$$\hat{w}_1 = 1$$

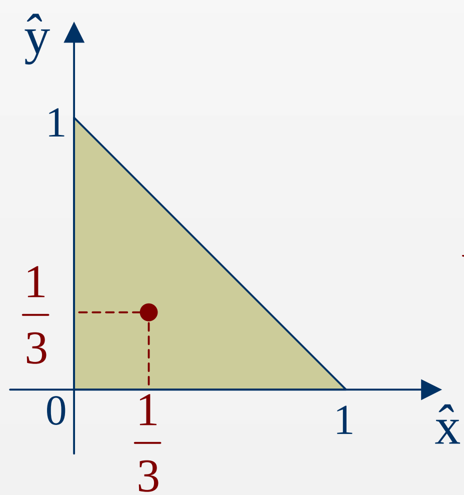
d=1 in the triangle

3 equations → 1 point, 1 weight



Mathematical problem - Physical interpretation

$$\begin{cases} \int_{\hat{e}} 1 \, dx \, dy = \frac{1}{2} = w_1 \\ \int_{\hat{e}} x \, dx \, dy = \frac{1}{6} = w_1 \hat{x}_1 \\ \int_{\hat{e}} y \, dx \, dy = \frac{1}{6} = w_1 \hat{y}_1 \end{cases}$$



$$\hat{w}_1 = \frac{1}{2}$$

d=2 in the square

6 equations → 2 points, 2 weights

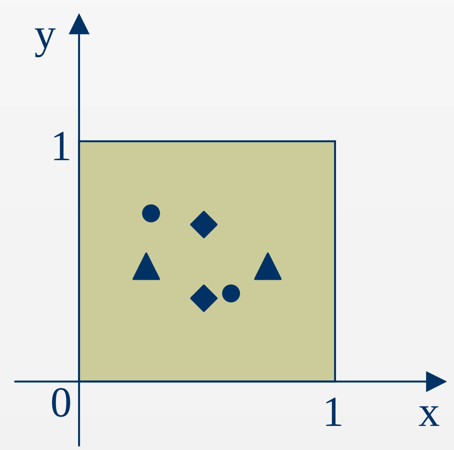
1
x — y
x^2 — xy — y^2

Mathematical problem - Physical interpretation

$$\int_{\hat{e}} 1\,dx\,dy = 1 = w_1 + w_2 \qquad \int_{\hat{e}} x^2 dx\,dy = \frac{1}{3} = w_1 \hat{x}_1^2 + w_2 \hat{x}_2^2$$

$$\int_{\hat{e}} x\,dx\,dy = \frac{1}{2} = w_1 \hat{x}_1 + w_2 \hat{x}_2 \qquad \int_{\hat{e}} y^2 dx\,dy = \frac{1}{3} = w_1 \hat{y}_1^2 + w_2 \hat{y}_2^2$$

$$\int_{\hat{e}} y\,dx\,dy = \frac{1}{2} = w_1 \hat{y}_1 + w_2 \hat{y}_2 \qquad \int_{\hat{e}} xy\,dx\,dy = \frac{1}{4} = w_1 \hat{x}_1 \hat{y}_1 + w_2 \hat{x}_2 \hat{y}_2$$



...no Mathematica solution…

d=3 (e.g. in the triangle)

10 equations → how many points?

3 points → too many equations?

4 points → not enough

$$
\begin{array}{ccccccc}
 & & & 1 & & & \\
 & & x & — & y & & \\
 & x^2 & — & xy & — & y^2 & \\
x^3 & — & x^2y & — & xy^2 & — & y^3
\end{array}
$$

Biquadratic polynomials for the square

- Let's choose two monomials p(x) and q(y) and let them be of degree d at most.

$$\begin{array}{ccccccc}
y^3 & — & xy^3 & — & x^2y^3 & — & x^3y^3 \\
| & & | & & | & & | \\
y^2 & — & xy^2 & — & x^2y^2 & — & x^3y^2 \\
| & & | & & | & & | \\
y & — & xy & — & x^2y & — & x^3y \\
| & & | & & | & & | \\
1 & — & x & — & x^2 & — & x^3
\end{array}$$

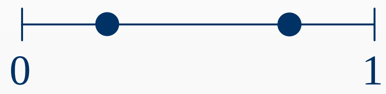
- If we choose d=3

- 16 equations → 4 points, 4 weights

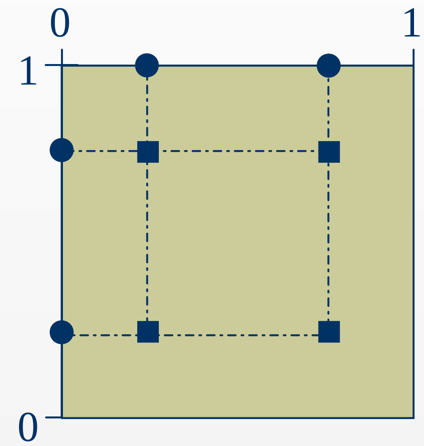
...no Mathematica solution (in a reasonable time)…

Cross product Gauss

Gauss 1D in [0,1]



Gauss 2D in $[0,1]^2$

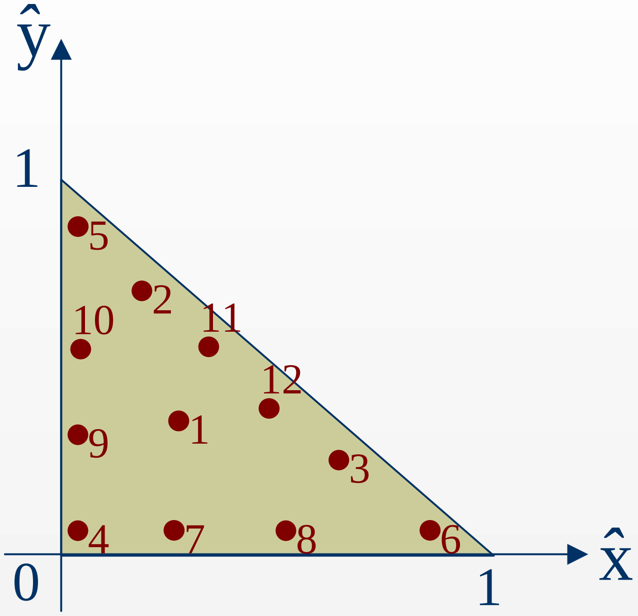


- only for domains like $[a,b]^n$

$$\iint g(x,y)\,dxdy = \int \sum_i w_i g(\hat{x}_i, y)\, dy = \sum_i w_i \int g(\hat{x}_i, y)\, dy = \sum_i \sum_j w_i w_j g(\hat{x}_i, \hat{x}_j)$$

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!



D.A.Dunuvant, HIGH DEGREE EFFICIENT SYMMETRICAL GAUSSIAN QUADRATURE RULES FOR THE TRIANGLE, International Journal for Numerical Methods in Engineering, vol. 21, **1129-1148** (1985)

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

Summary

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

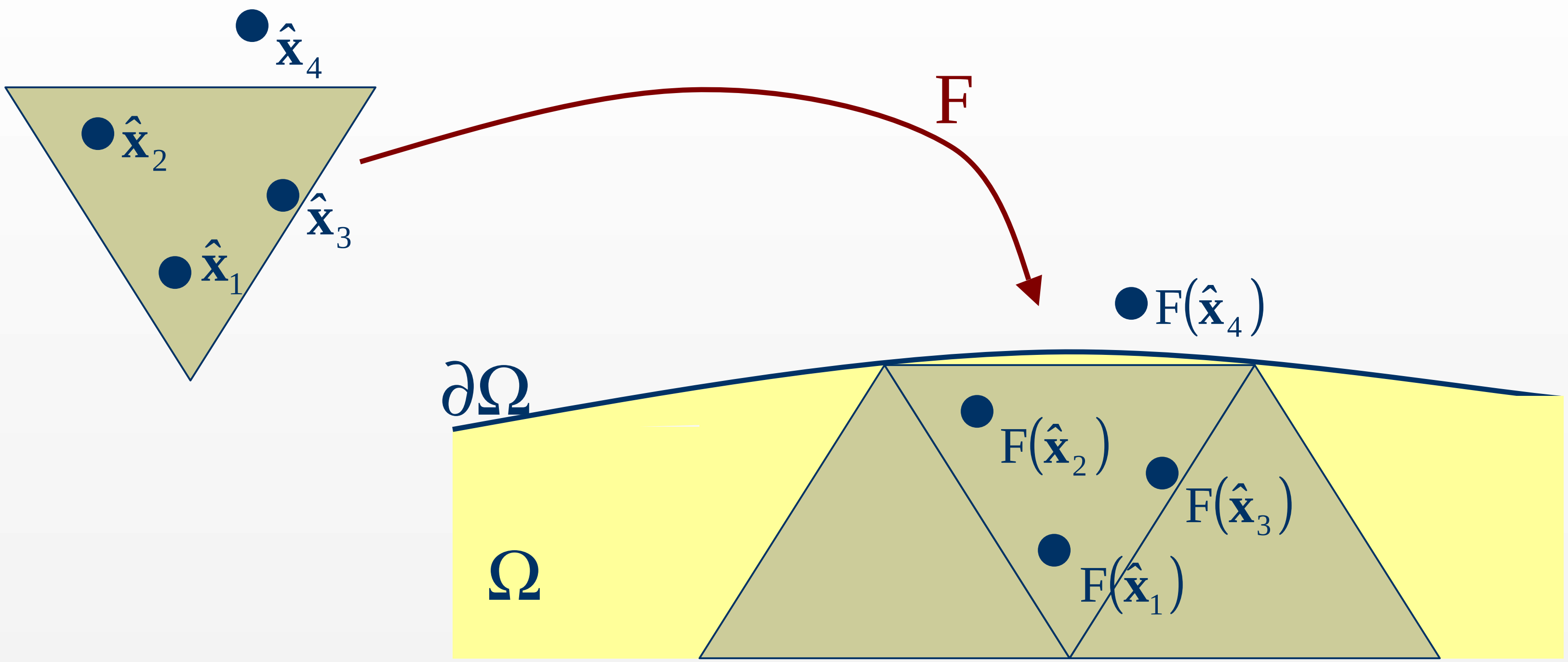
Does the non-linear system have a solution?

Is the found solution acceptable?

WE HAVE AN ACCEPTABLE QUADRATURE METHOD!

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

Condition 1: $\hat{x}_i \in \hat{e} \ \forall i$



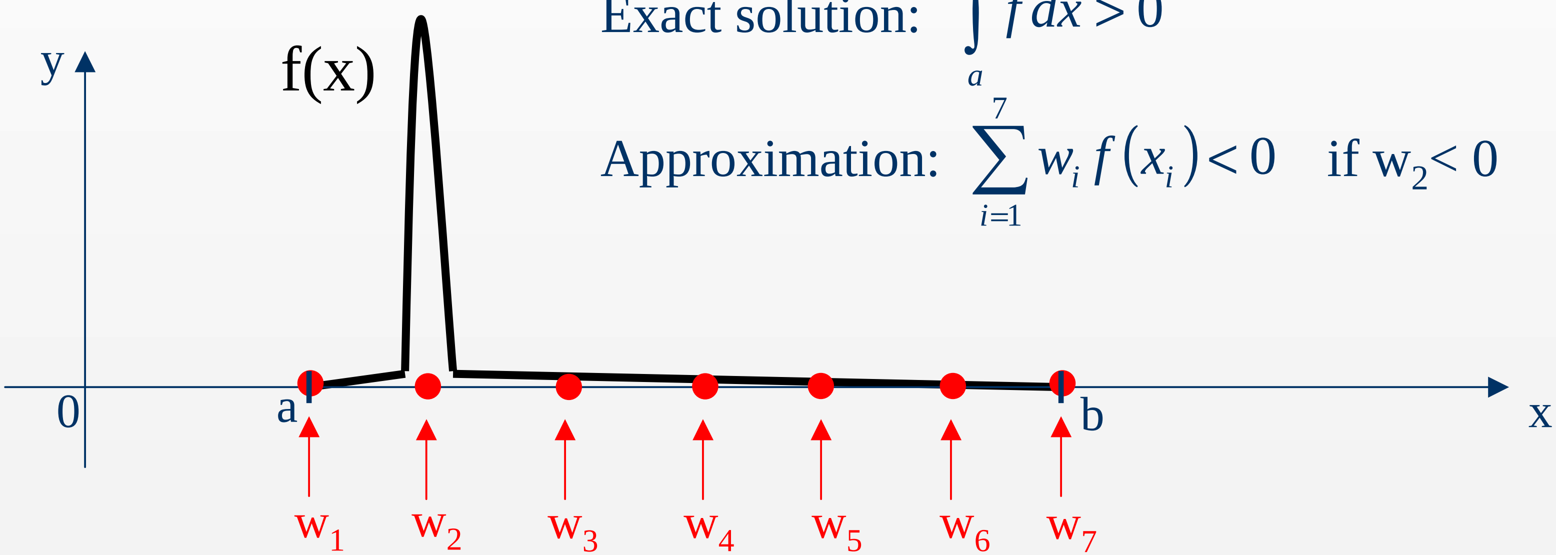
What is the value of $f(F(\hat{\mathbf{x}}_4))$ if $F(\hat{\mathbf{x}}_4)$ does not belong to Ω?

Condition 2: $w_i \geq 0, \forall i$

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

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

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



- Finite Elements Methods (FEM)

Why weights always ≥ 0 in FEM

- Stiffness matrix **A** is positive definite

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

$$\mathbf{u} = [\mathrm{u}_1, \ldots, \mathrm{u}_n] \rightarrow \ \mathrm{u} = \sum_i \mathrm{u}_i \varphi_i \qquad \mathrm{a}_{ij} = \int \left(\nabla \varphi_j \nabla \varphi_i + \varphi_j \varphi_i\right) \mathrm{d}\mathbf{x}$$

- 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]:

n	A_1	A_2	A_3	A_4	A_5	A_6
1	$\frac{1}{2}$					
3	$\frac{1}{3}$	$\frac{4}{3}$				
9	$\frac{989}{14175}$	$\frac{5888}{14175}$	$-\frac{928}{14175}$	$\frac{10496}{14175}$	$-\frac{4540}{14175}$	
11	$\frac{16067}{299376}$	$\frac{106300}{299376}$	$-\frac{48525}{299376}$	$\frac{272400}{299376}$	$-\frac{260550}{299376}$	$\frac{427368}{299376}$

- Negative weights also in many formula using with Gauss approach

Covering

- Example 2: triangles → more flexible