Is integration in 2D or 3D really different from integration in 1D?

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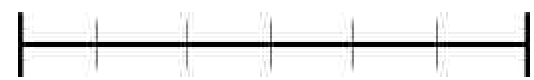
Overview

- Numerical integration in 1D
- Numerical integration in xD
- Literature
- Available software

Numerical integration

1. Partition complex region into fundamental ones

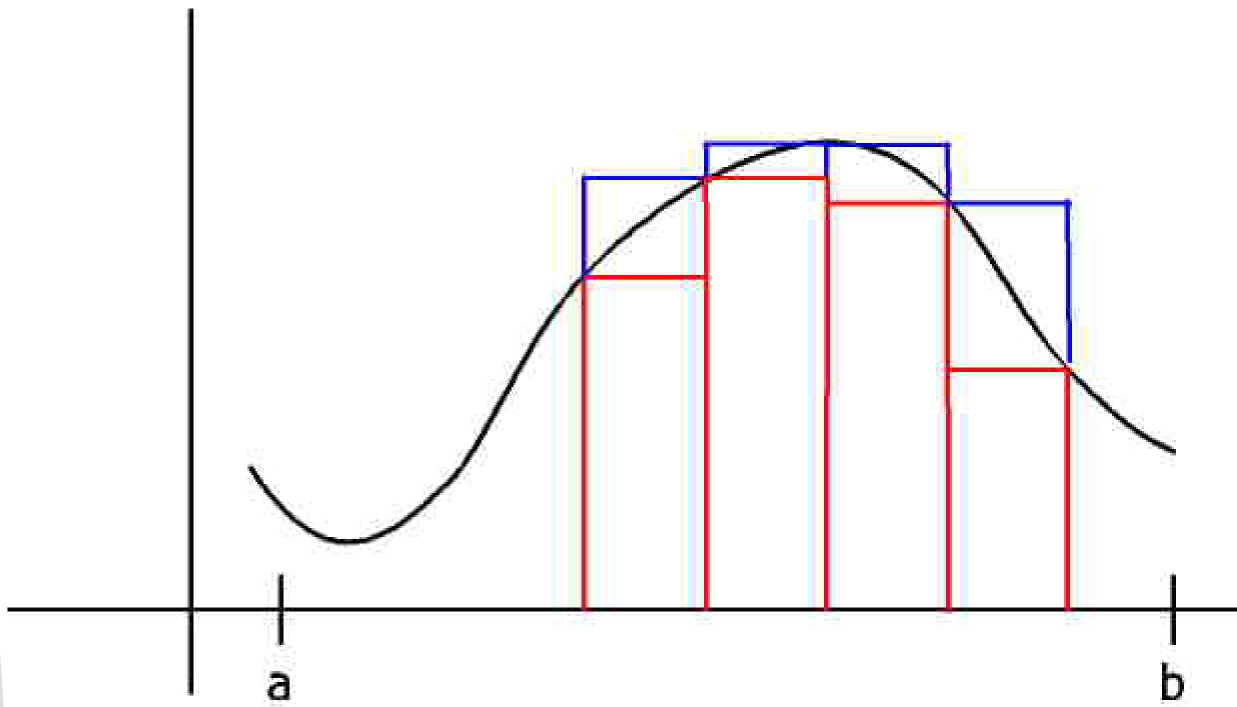


2. Use numerical integration on fundamental region

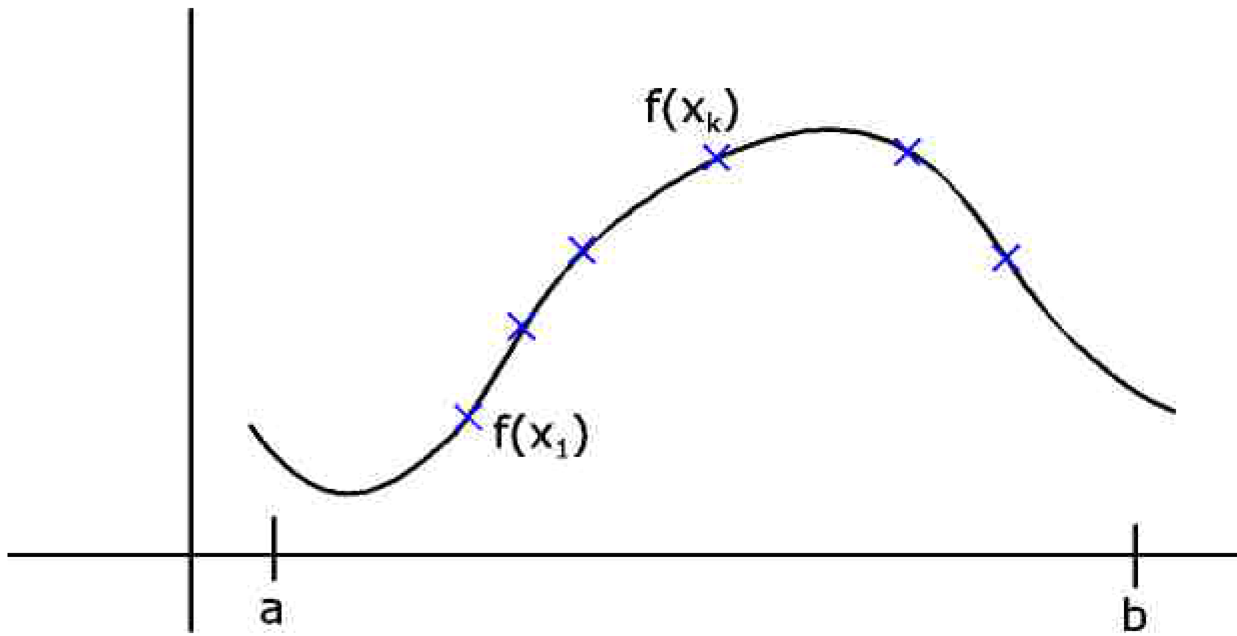
3. Adaptive: let partition depend on function

Riemann integration

- Approximation:



Monte Carlo



$$\int_{\Omega} f = \frac{1}{N} \sum_{k=1}^{N} f(x_k)$$

Errors

1. In basic region, due to approximation error

2. Error due to non-exact covering of the region with basic regions

Num. Integration of Basic Regions

- Standard

$$\int f \doteq \sum_i w_i f(x_i)$$

- Advanced

$$\int f \doteq \sum_k \sum_p w_{k,p} f^{(p)}(x_k)$$

Degrees of freedom: w_k and x_k

Error

- A rule is called *exact* for $f(x)$ if the error, given by $\int f - \sum w_k f(x_k)$ is zero.

- A rule is *exact for degree n* if it is exact for polynomials of degree up to n and not for $n+1$

The best integration rule

- Minimal amount of points, such that the rule is exact for specific degree p

Rules for integration

1. Choose x_k determine w_k: Newton-Cotes (demand degree p exact)
2. Interpolate the function $f(x) \doteq \sum_{k=1}^{n} \alpha_i(f) g_i(x)$ then:

$$\int f(x) \doteq \int \sum_{i=1}^{n} \alpha_i(f) g_i(x) = \sum_{i=1}^{n} \alpha_i(f) \int g_i(x)$$

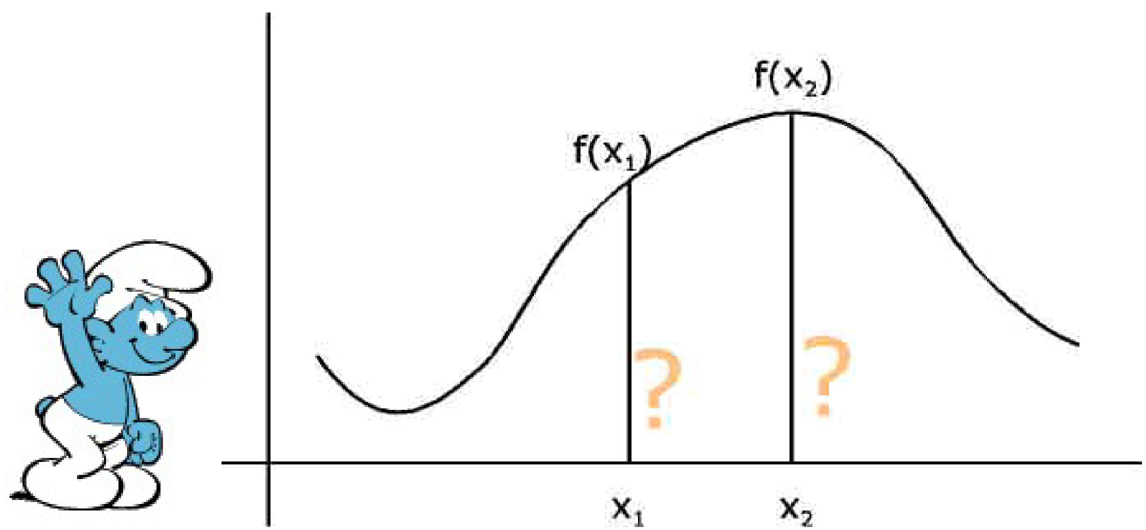
3. Determine x_k and w_k: Gauss-Legendre (demand degree p exact)

Rules for integration

- Newton-Cotes via interpolation
  - Error also via interpolation error
- Gauss-Legendre via orthogonal polynomials
  - Error also via orthogonal polynomials

Examples

- Newton-Cotes
- Gauss-Legendre



Orthogonal polynomials

Integration over interval [a,b]

- The optimal points are the zeros of the orthogonal polynomial $P_n(x)$ on [a,b].

  $$\int_a^b P_n(x) Q_{n-1}(x)\,dx = 0$$

  for all polynomials $Q_{n-1}(x)$ of degree $\leq$n-1.

Proof in [1]

Proof

[1] A.H. Stroud " Numerical Quadrature and Solution of Ordinary Differential Equations"

$$\int_a^b P_n(x)Q_{n-1}(x)dx = 0 = \sum w_k P_n(x_k)Q_{n-1}(x_k)$$

$$\Rightarrow P_n(x_k) = 0$$

and

$$\int Q_{2n-1}(x)dx = \sum A_k Q_{2n-1}(x_k) \quad \text{exact}$$

$$\underbrace{\int S_{n-1}(x)\,dx}_{\text{exact}} + \underbrace{\int P_n(x)R_{n-1}(x)dx}_{0}$$

Orthogonal polynomials

- It can be proven that:
  - $P_n(x)$ is unique (normalized)
  - That zeros are real and distinct and lie in the open interval (a,b)
  - Zeros distributed symmetrically?
- $P_n(x)$ can be found efficiently via recursion relation.

$$P_n(x) = (x - \beta_n) P_{n-1}(x) - \gamma_n P_{n-2}(x)$$

$$P_1(x) = x - \beta_1 \quad P_0(x) = 1$$

Error Newton-Cotes

- Error made with Newton-Cotes can be determined with the interpolation error:

$$f(x) - p_f(x) = (x - x_1)\ldots(x - x_n)\frac{f^{(n)}(\xi)}{n!}$$

so:

$$\int f(x) - \int p_f(x) = \int (x - x_1)\ldots(x - x_n)\frac{f^{(n)}(\xi)}{n!}$$

Error Gauss-Legendre

- Also: weights are positive
- The error made for arbitrary *f(x)* for a simple region:

$$R(f) = I(f) - \sum_{i=1}^{n} w_i f(x_i) =$$

$$\frac{1}{(2n)!} f^{(2n)}(\theta) \int_a^b (P_n(x))^2 dx = cf^{(2n)}(\theta)$$

Integration in 2D

- For basic regions some formulae exist or can be determined from 1D method
- Fundamental geometries

- For non-trivial regions:
  - Use Monte Carlo
  - Partition into basic regions

Lagrange for basic region in *x*D

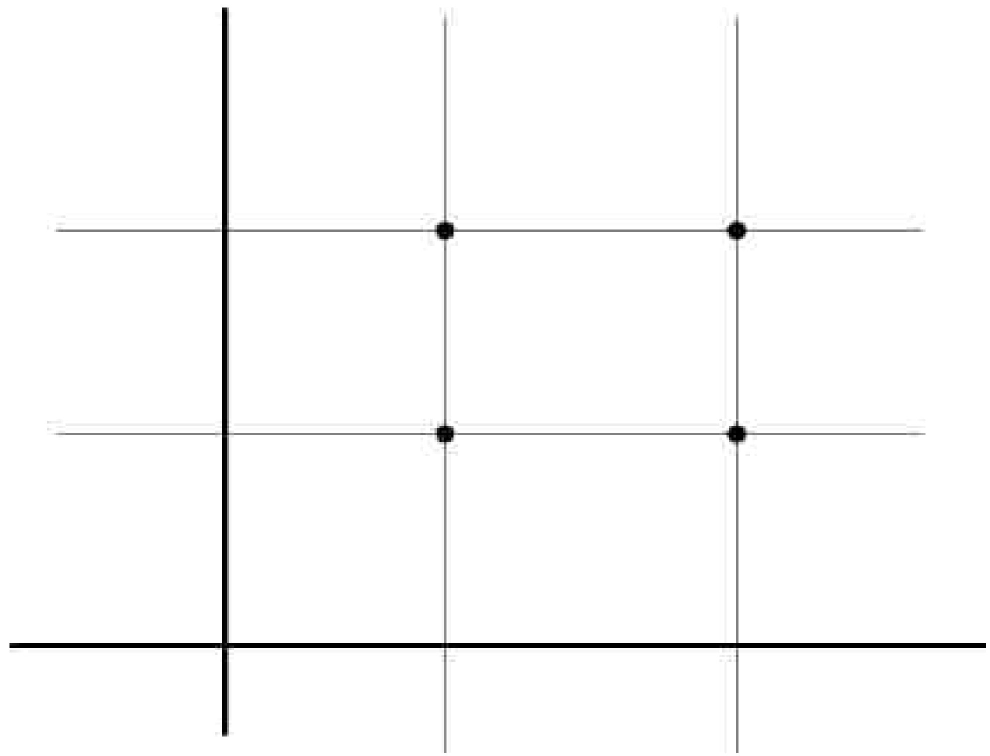
- Let two Lagrangian polynomials be given:

$$L_n(f,x)=\sum_{i=1}^{n}\lambda_i(x)f(x_i,y),\quad L_m(f,y)=\sum_{j=1}^{m}\mu_j(y)f(x,y_j)$$

- Then the 2-dimensional interpolating function:

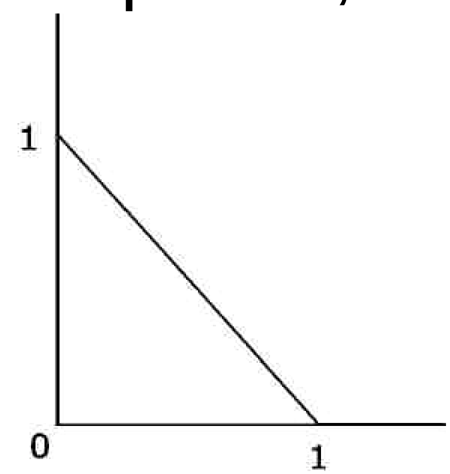
$$\mathbf{L}_{nm}(f,x,y)\equiv L_n(L_m(f,x),y)=\sum_{i=1}^{n}\sum_{j=1}^{m}\lambda_i(x)\mu_j(y)f(x_i,y_j)$$

Lagrange for basic region in *x*D



Newton-Cotes for basic region in xD

- For simple domains only
- Domain specific, example simplex



- Newton-Cotes cubatures can be found via cardinal functions [3]

Newton-Cotes for basic region in *x*D

- Cardinal functions:

$$\lambda_{1,1}(x,y) = -(x+y-1), \quad \lambda_{1,2}(x,y) = x, \quad \lambda_{1,3}(x,y) = y,$$

- Interpolating

$$L_1(f,x,y) = (1-x-y)\ f(0,0) + x\ f(1,0) + y\ f(0,1)$$

- Which leads to a first-degree rule

$$C_3 f = \int_0^1 \int_0^{1-x} L_1(f,x,y)\,dy\,dx = \frac{1}{6}[\ f(0,0) + f(1,0) + f(0,1)]$$

Given rules for 2D

- Stroud [2] gives some rules for a set of basic regions
  - Degree
  - Number of points
- With * are “particularly useful”

Given rules for 2D

- *-Example:

  $C_{2:}$5-1 degree 5, with 7 points:

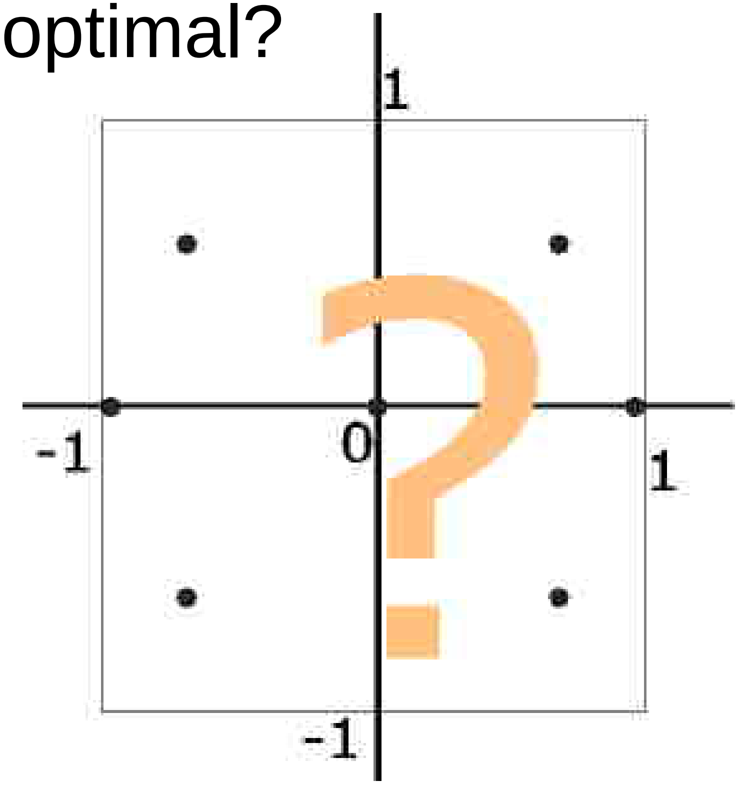
  $\left(\pm\sqrt{\frac{3}{5}},\pm\sqrt{\frac{1}{3}}\right)$ with weight $\frac{5}{36}V$

  $\left(0,\pm\sqrt{\frac{14}{15}}\right)$ with weight $\frac{5}{63}V$

  $(0,0)$ with weight $\frac{2}{7}V$

The optimal choice?

- Problem remains: is the choice of your points optimal?



Gauss for ***x***D

- Zeros of ***x***D-orthogonal polynomials
- Example 2D:
- Square $|x|, |y| \leq 1$. Find cubature rule with degree 2.
- Orthogonal polynomials can be found:

$$p^{(2,0)}(x,y) = x^2 - \frac{1}{3} \quad p^{(1,1)}(x,y) = xy \quad p^{(0,2)}(x,y) = y^2 - \frac{1}{3}$$

- But, how many points to choose?

Open problem

Given a fundamental geometry

Then find the least amount of points (and weights) such that

$$\int_{\hat{e}} f \doteq \sum_i w_i f(x_i)$$

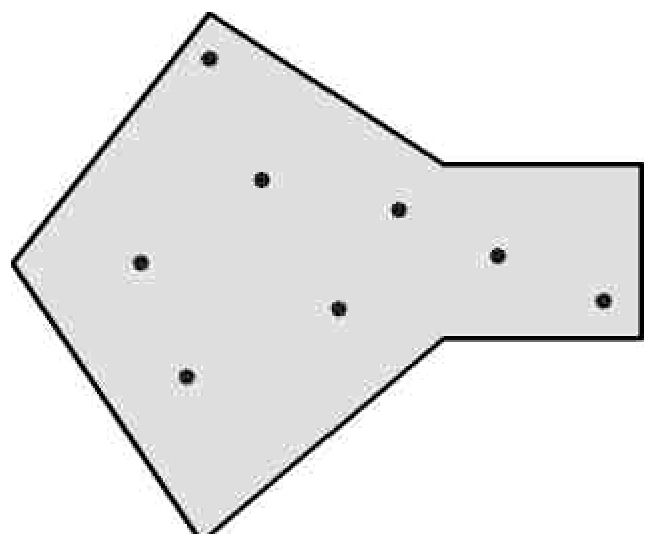
is exact for degree d.

Next session more about this problem

Monte Carlo approach

- First order method: $\int_{\Omega} f = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$

  with N randomly chosen numbers



Literature

Library (CUL):

[1] A.H. Stroud " *Numerical Quadrature and Solution of Ordinary Differential Equations*",1974

[2] A.H. Stroud, "*Appr. Calculation of Multiple Integrals*", 1971

[3] H. Engels, *"Numerical Quadrate and Cubature*", 1980

Articles:

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@ARTICLE{AllgGeor4,
 AUTHOR="E. Allgower, K. Georg and R. Widmann",
 TITLE="Volume integrals for boundary element methods",
 JOURNAL="Journal of Computational and Applied Mathematics",
 PAGES="17--29",
 VOLUME="38",
 YEAR="1991"}

@ARTICLE{CooRab,
 AUTHOR="R. Cools and P. Rabinowitz",
 TITLE="Monomial cubature rules since ``Stroud'': a compilation",
 JOURNAL="Journal of Computational and Applied Mathematics",
 PAGES="309--326",
 VOLUME="48",
 YEAR="1993"}

@ARTICLE{Duve,
 AUTHOR="D.A.~Dunavant",
 TITLE="High degree efficient symmetric gauss quadrature rules for the
    triangle",
 JOURNAL="International Journal for Numerical Methods in Engineering",
 PAGES="1129--1148",
 VOLUME="21",
 YEAR="1985"}

@ARTICLE{GeorWidm,
 AUTHOR="K. Georg and R. Widmann",
 TITLE="Adaptive quadratures over volumes",
 JOURNAL="Computing",
 PAGES="121--136",
 VOLUME="47",
 YEAR="1991"}
```

```
@ARTICLE{Grund78,
 AUTHOR="Axel Grundmann and H.M. M\"oller",
 TITLE="Invariant integration formulas for the n-simplex by combinatorial methods",
 JOURNAL="SIAM J. Numer. Anal.",
 VOLUME="15",
 NUMBER="2",
 PAGES="282-290",
 YEAR="1978"}

@ARTICLE{Kaha91,
 AUTHOR="D.K. Kahaner",
 TITLE="A Survey of Existing multidimensional quadrature
 Routines",
 JOURNAL="Contemporary Mathematics",
 VOLUME="155",
 YEAR="1991"}

@BOOK{Reich,
 AUTHOR="S. Reich",
 BOOKTITLE="Backward Error Analysis for Numerical Integrators",
 YEAR="1996",
 PUBLISHER="Preprint SC of the Konrad Zuse-Zentrum f\umlaut ur Informationstechnik Berlin,
    Berlin, October Germany”}

@BOOK{Zumb1,
 AUTHOR="G. W. Zumbusch",
 BOOKTITLE="Adaptive h-p approximation procedures, graded meshes and anisotropic refinement
    for Numerical Quadrature",
 YEAR="1995",
 PUBLISHER="Preprint SC of the Konrad Zuse-Zentrum f\umlaut ur Informationstechnik Berlin,
    Berlin, October Germany“}
```

Available software

- NAG-Lib
- QUADPACK
- Net-lib
- Mathematica
  - Packages:
    - **`NumericalMath`GaussianQuadrature``**
    - **`NumericalMath`NewtonCotes``**
    - **More…**
  - **Normally Gauss-Konrod based**
- Matlab

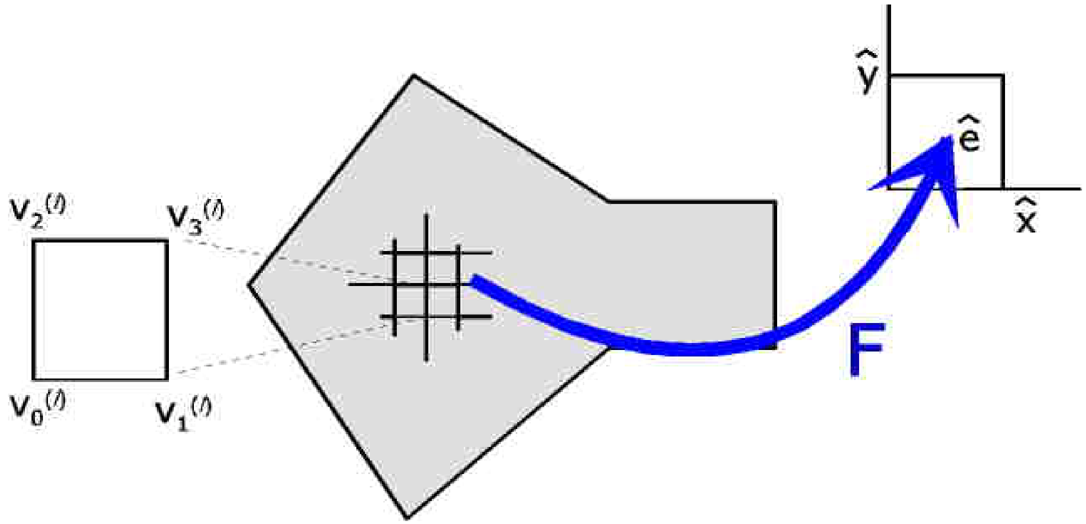
The answer is….

Yes!

Integrating in 2D or 3D **is** really different from integrating in 1D!

Map to fundamental geometry

- The domain Ω is divided into elements:



$$F_l\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} = \begin{bmatrix} v_1^{(l)} - v_0^{(l)} & v_2^{(l)} - v_0^{(l)} \end{bmatrix}\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix} + v_0^{(l)}$$

Domain Decomposition

- Integration per element:

$$\int_{e_l} f(x)dx = \int_{\hat{e}} f(F_l(\hat{x})) \left|\det(\partial F_l(\hat{x}))\right| d\hat{x}$$

- Assume a given quadrature rule:

$$\int_{\hat{e}} g(\hat{x})d\hat{x} \doteq \sum_i w_i g(\hat{x}_i)$$

- Then: $\int_{e_l} f(x)dx = \left|\det(\partial F_l(\hat{x}))\right| \sum_i w_i f(F_l(\hat{x}_i))$

$\left|\det(\partial F_l(\hat{x}))\right|$ is a number dependent on the element.