Lecture 23

Integration: Gauss Quadrature

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Today:

Finishing

- Newton Cotes Methods

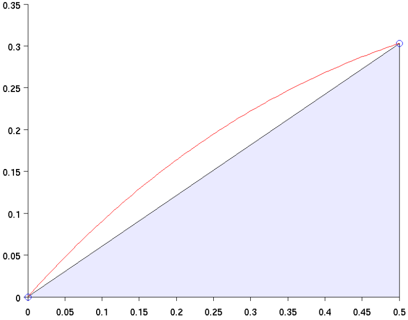
Moving Forward

- Identify the most widely used quadrature method
- Is it cheap?
- Is it effective?
- How does it compare to Newton-Cotes (Trapezoid, Simpson, etc)?

Basic Trapezoid

Use endpoints $[a, b]$ to obtain a linear approximation to $f(x)$. The area under this function is the area of a trapezoid:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)(f(a)+f(b))$$

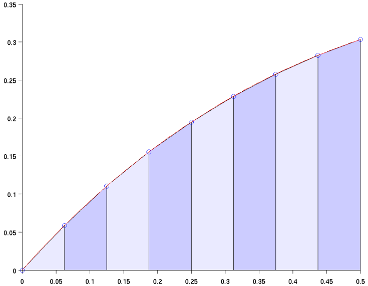


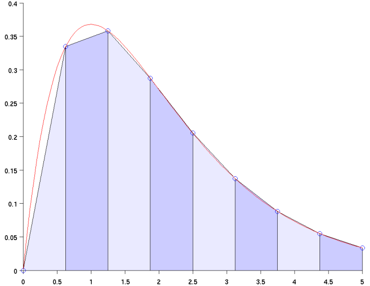
Trapezoid

Composit Trapezoid

In each interval $[x_i, x_{i+1}]$, use the basic Trapezoid:

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} \frac{1}{2}(x_{i+1} - x_i)(f(x_i) + f(x_{i+1}))$$



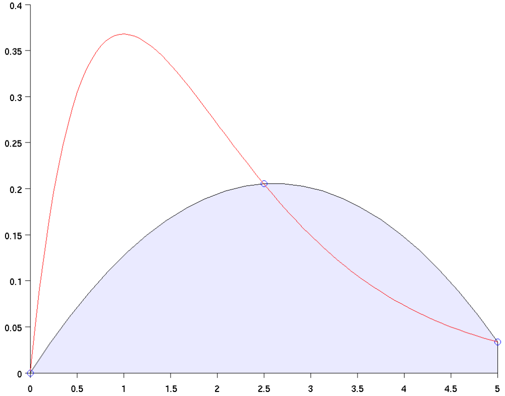


Simpson

Since $b - a = 2h$ we have

Basic Simpson's Rule

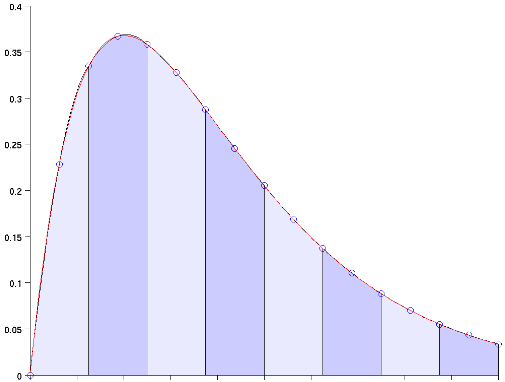
$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$



Simpson

Composite Simpson's Rule

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(a) + f(b) + 4\sum_{i=1}^{n/2} f(a + (2i-1)h) + 2\sum_{i=1}^{n/2-1} f(a + 2ih)\right]$$



Summary

Summary:

- Left/Right Riemann: approximate $f(x)$ by 0-degree $p(x)$ and integrate
- Trapezoid: approximate $f(x)$ by 1-degree $p(x)$ and integrate
- Simpson: approximate $f(x)$ by 2-degree $p(x)$ and integrate
  (note: our proof showed that Simpson is "perfect" for cubic polynomials as well!)

Note, for basic methods, we've assumed that evaluation points are evenly spaced.

Newton-Cotes

Definition: Newton-Cotes integration rules use evenly spaced points on the interval $[a, b]$

Basic Newton-Cotes rules:

name	n	formula
Trapezoid	1	$\frac{(b-a)}{2}\left[f(a)+f(b)\right]$
Simpson's 1/3	2	$\frac{(b-a)}{6}\left[f(a)+4f(\frac{a+b}{2})+f(b)\right]$
Simpson's 3/8	3	$\frac{(b-a)}{8}\left[f(a)+3f(a+h)+3f(b-h)+f(b)\right]$
Boole's	4	$\frac{(b-a)}{90}\left[7f(a)+32f(a+h) + 12f(\frac{a+b}{2})+32f(b-h)+7f(b)\right]$

Newton-Cotes

Error bounds for composite Newton-Cotes:

name	n	error	h
Trapezoid	1	$-\frac{(b-a)h^2}{12}f''(\xi)$	$h = b - a$
Simpson's $1/3$	2	$-\frac{(b-a)h^4}{90}f^{(4)}(\xi)$	$h = (b-a)/2$
Simpson's $3/8$	3	$-\frac{(b-a)h^4}{80}f^{(4)}(\xi)$	$h = (b-a)/3$
Boole's	4	$-\frac{2(b-a)h^6}{945}f^{(6)}(\xi)$	$h = (b-a)/4$

Changing Gears

And now for a change of perspective.

Degree of Precision

Degree of Precision

If integration rule has zero error when integrating any polynomial of degree $\leqslant r$
AND
If the error is nonzero for some polynomial of degree $r + 1$,

Then, the rule has *degree of precision* **equal to** r.

- Trapezoid rule has degree of precision $= 1$
  (Error = $-\dfrac{(b-a)h^2 f''(\eta)}{12} = 0$ for linear polynomials).
- Simpson's rule has degree of precision $= 3$, because the error $\sim f^{(4)}$
- Even though we integrated a quadratic in deriving Simpson's rule, it can integrate cubics exactly!
- Can we extend this idea, and use a quadratic interpolant to derive an even higher degree rule?

Quadrature

Numerical Quadrature: Integration rules $\sum_{i=1}^{n} w_i f(x_i) \approx \int_a^b f(x)\,dx$

- So far, our quadrature methods were of the form

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j)$$

  with equally space points x_j, and weights w_j
- Trapezoid:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b) = w_0 f(a) + w_1 f(b)$$

- Simpson:

$$\begin{aligned}\int_a^b f(x)\,dx \approx & \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b) \\ = & w_0 f(a) + w_1 f\left(\frac{a+b}{2}\right) + w_2 f(b)\end{aligned}$$

- Similar for higher order polynomial Newton-Cotes rules

Quadrature with Freedom

!

These quadrature rules have one thing in common: they're restrictive

- For example, Simpson's:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b)$$

- Trapezoid, Simpson, etc (Newton-Cotes) use equally spaced points
- We know one thing already from interpolation: equally spaced nodes result in *wiggle*.
- What other choice do we have? (...recall how we fixed wiggle in interpolation: by moving the location of the nodes)

Gaussian Quadrature

- Free yourself! (from equally spaced nodes)
- Combine selection of the nodes and selection of the weights into one quadrature rule

Gaussian Quadrature

Choose the nodes and coefficients optimally to maximize the degree of precision of the quadrature rule:

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j)$$

Goal

Seek w_j and x_j so that the quadrature rule is exact for really high polynomials

Gaussian Quadrature

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j)$$

- We have $n+1$ points $x_j \in [a,b]$, $a \leqslant x_0 < x_1 < \cdots < x_{n-1} < x_n \leqslant b$.
- We have $n+1$ real coefficients w_j

- So there are $2n+2$ total unknowns to take care of

- There were only 2 unknowns in the case of trapezoid (2 weights)
- There were only 3 unknowns in the case of Simpson (3 weights)
- There were only $n+1$ unknowns in the case of general Newton-Cotes ($n+1$ weights)

Gaussian Quadrature

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$2n+2$ unknowns (using $n+1$ nodes) can be used to exactly interpolate and integrate polynomials of degree up to $2n+1$

Better Nodes Example

The first thing we do is SIMPLIFY

- Consider the case of $n = 1$ (2-points)
- Consider $[a, b] = [-1, 1]$ for simplicity
- We *know* how the trapezoid rule works
- Question: can we possibly do better using only 2 function evaluations?
- Goal: Find w_0, w_1, x_0, x_1 so that

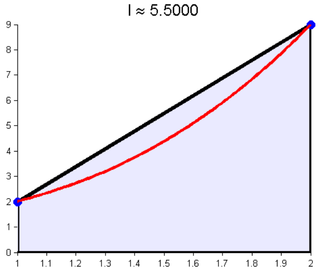
$$\int_{-1}^{1} f(x)\,dx \approx w_0 f(x_0) + w_1 f(x_1)$$

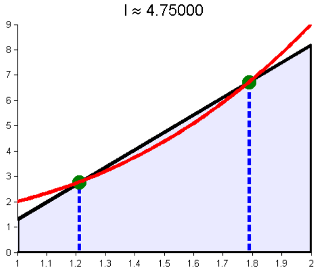
  is as accurate as possible...

Graphical View

Consider

$$\int_1^2 x^3 + 1 \, dx = 4.75$$





Derive...

Again, we are considering $[a, b] = [-1, 1]$ for simplicity:

$$\int_{-1}^{1} f(x)\ dx \approx w_0 f(x_0) + w_1 f(x_1)$$

Goal: find w_0, w_1, x_0, x_1 so that the approximation is exact up to cubics. So, we consider any arbitrary cubic:

$$f(x) = a + bx + cx^2 + dx^3$$

This implies that:

$$\begin{aligned}
\int_{-1}^{1} f(x)\ dx &= \int_{-1}^{1} \left(a + bx + cx^2 + dx^3\right)\ dx \\
&= w_0 \left(a + bx_0 + cx_0^2 + dx_0^3\right) + \\
&\quad\ w_1 \left(a + bx_1 + cx_1^2 + dx_1^3\right)
\end{aligned}$$

Derive...

$$\begin{aligned}\int_{-1}^{1} f(x)\, dx &= \int_{-1}^{1} \left(a + bx + cx^2 + dx^3\right)\, dx \\ &= w_0\left(a + bx_0 + cx_0^2 + dx_0^3\right) + \\ &\quad\; w_1\left(a + bx_1 + cx_1^2 + dx_1^3\right)\end{aligned}$$

Rearrange:

$$a\left(w_0 + w_1 - \int_{-1}^{1} dx\right) + b\left(w_0x_0 + w_1x_1 - \int_{-1}^{1} x\, dx\right) +$$
$$c\left(w_0x_0^2 + w_1x_1^2 - \int_{-1}^{1} x^2\, dx\right) + d\left(w_0x_0^3 + w_1x_1^3 - \int_{-1}^{1} x^3\, dx\right) = 0$$

Since a, b, c and d are arbitrary, then their coefficients must all be zero.

Derive...

This implies:

$$w_0 + w_1 = \int_{-1}^{1} dx = 2 \qquad w_0 x_0 + w_1 x_1 = \int_{-1}^{1} x \, dx = 0$$

$$w_0 x_0^2 + w_1 x_1^2 = \int_{-1}^{1} x^2 \, dx = \frac{2}{3} \qquad w_0 x_0^3 + w_1 x_1^3 = \int_{-1}^{1} x^3 \, dx = 0$$

Four equations, four unknowns, solution is:

$$w_0 = 1 \quad w_1 = 1 \quad x_0 = -\frac{\sqrt{3}}{3} \quad x_1 = \frac{\sqrt{3}}{3}$$

Therefore:

$$\int_{-1}^{1} f(x) \, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

Over another interval?

$$\int_{-1}^{1} f(x)\, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

$$\int_{a}^{b} f(x)\, dx \approx ?$$

- Integrating over $[a, b]$ instead of $[-1, 1]$ needs a transformation: a change of variables
- Let $x(t) = \dfrac{b-a}{2} t + \dfrac{b+a}{2}$
- Verify that $x(t = -1) = a$ and $x(t = 1) = b$
- Then $dx = \dfrac{b-a}{2} dt$

Notes

To the board

Over another interval?

$$\int_a^b f(x)\,dx \approx ?$$

- Let $x(t) = \frac{b-a}{2}t + \frac{b+a}{2}$
- Then $dx = \frac{b-a}{2}dt$

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)t}{2} + \frac{b+a}{2}\right)\frac{b-a}{2}\,dt$$

- Now use the quadrature formula over $[-1, 1]$

Extending Gauss Quadrature

- Remember, we constructed our 2-point ($n = 1$) Gauss quadrature rule to give us exact integration for polynomials of degree 2*1+1 = 3, and less.
- We need more to make this work for more than two points
- Note: one sensible quadrature rule for the interval $[-1, 1]$ based on 1 node would use the node $x = 0$. Any other x value would *over-weight* one side of the interval $[-1, 1]$. This is a root of $\phi(x) = x$.
- Note: $\pm\frac{1}{\sqrt{3}}$ are the roots of $\phi(x) = 3x^2 - 1$
- What about general $\phi(x)$?

Gauss Quadrature Theorem

Karl Friedrich Gauss proved the following result:
Let $q(x)$ be a nontrivial polynomial of degree $n+1$ such that

$$\int_a^b x^k q(x)dx = 0 \qquad (0 \leqslant k \leqslant n)$$

and let $x_0, x_1, \ldots, x_n$ be the zeros of $q(x)$. Then

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i), \text{ where } w_i = \int_a^b \ell_i(x)dx$$

will be exact for all polynomials of degree at most $2n+1$. (Wow!)

(Recall $\ell_i(x)$ is the ith Lagrange basis function. Here, $\ell_i(x)$ is defined with respect to the $x_0, x_1, \ldots, x_n$ zeros of $q(x)$.)

Notes

Sketch of Proof

1. Let $f(x)$ be any polynomial of degree $2n+1$. Then we can write $f(x) = p(x)q(x) + r(x)$, where $p(x)$ and $r(x)$ are of degree at most n

  - This is basically dividing f by q with remainder r.

2. Then by the hypothesis, $\int_a^b p(x)q(x)dx = 0$. Thus,

$$\int_a^b f(x)dx = \int_a^b r(x)dx = \sum_{i=0}^{n} r(x_i)\int_a^b \ell_i(x)dx = \sum_{i=0}^{n} f(x_i)\int_a^b \ell_i(x)dx$$

  - Here we used the fact that since $r(x)$ is (at most) a degree n polynomial,
  we can represent $r(x) = \sum_{i=0}^{n} r(x_i)\ell_i(x)$.

  - And lastly, we use the fact that $f(x_i) = p(x_i)q(x_i) + r(x_i) = r(x_i)$, because $q(x_i) = 0$ at each of it's zeros x_i

Thus, we need to find the polynomials $q(x)$. The terms $\int_a^b \ell_i(x)dx$ will be our quadrature weights, and the x_i will be our quadrature nodes.

Orthogonal Polynomials

Orthogonality of Functions

Two functions $g(x)$ and $h(x)$ are *orthogonal* on $[a, b]$ if

$$\int_a^b g(x)h(x)\,dx = 0$$

- So, the nodes we're using are roots of orthogonal polynomials
- These are the *Legendre* Polynomials

Legendre Polynomials

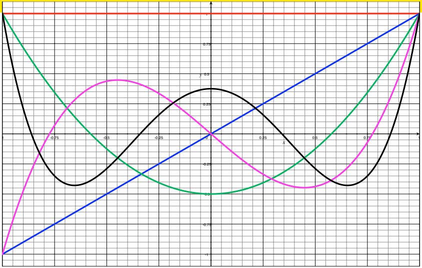
Do not memorize: given on the exam

$$\phi_0 = 1$$
$$\phi_1 = x$$
$$\phi_2 = \frac{3x^2 - 1}{2}$$
$$\phi_3 = \frac{5x^3 - 3x}{2}$$
$$\vdots$$

In general:

$$\phi_n(x) = \frac{(2n-1)x}{n}\phi_{n-1}(x) - \frac{n-1}{n}\phi_{n-2}(x)$$

Notes on Legendre Roots



- The Legendre Polynomials are orthogonal (nice!)
- The Legendre Polynomials increase in polynomial order (like monomials), $\Rightarrow \phi_n$ is degree n polynomial
- The Legendre Polynomials don't suffer from poor conditioning (unlike monomials)
- The Legendre Polynomials don't have a closed form expression (recursion relation is needed)
- The roots of the Legendre Polynomials are the nodes for Gaussian Quadrature (GL nodes)

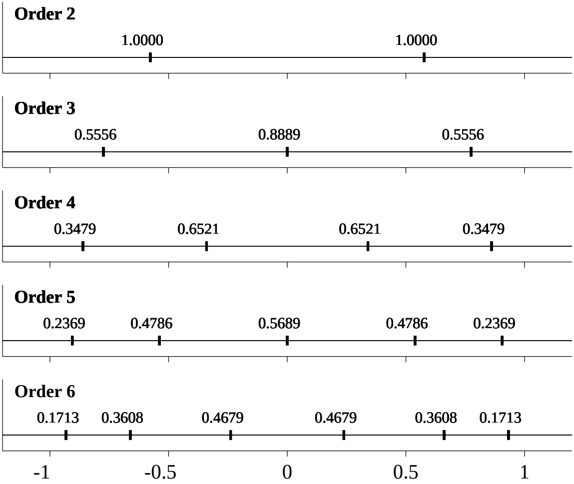
Quadrature Nodes (see)

- Often listed in tables
- Weights determined by extension of above
- Roots are symmetric in $[-1, 1]$
- Example:

```
if(n==0)
  x = 0;    w = 2;
if(n==1)
  x(1) = -1/sqrt(3);      x(2) = -x(1);
  w(1) =  1;              w(2) =  w(1);
if(n==2)
  x(1) = -sqrt(3/5);     x(2) =  0;       x(3) = -x(1);
  w(1) =  5/9;           w(2) =  8/9;     w(3) =  w(1);
if(n==3)
  x(1) = -0.861136311594053;     x(4) = -x(1);
  x(2) = -0.339981043584856;     x(3) = -x(2);
  w(1) =  0.347854845137454;     w(4) =  w(1);
  w(2) =  0.652145154862546;     w(3) =  w(2);
if(n==4)
  x(1) = -0.906179845938664;     x(5) = -x(1);
  x(2) = -0.538469310105683;     x(4) = -x(2);
  x(3) =  0;
  w(1) =  0.236926885056189;     w(5) =  w(1);
  w(2) =  0.478628670499366;     w(4) =  w(2);
  w(3) =  0.568888888888889;
if(n==5)
  x(1) = -0.932469514203152;     x(6) = -x(1);
  x(2) = -0.661209386466265;     x(5) = -x(2);
  x(3) = -0.238619186083197;     x(4) = -x(3);
  w(1) =  0.171324492379170;     w(6) =  w(1);
  w(2) =  0.360761573048139;     w(5) =  w(2);
  w(3) =  0.467913934572691;     w(4) =  w(3);
```

View of Gauss Integration Formulas

- Nodes are **thick** black hash marks (symmetric)
- Weights are given numerically above nodes (symmetric)



Theory

The connection between the roots of the Legendre polynomials and exact integration of polynomials is established by the following theorem.
(Extension of earlier Gauss quadrature theorem.)

Theorem

Suppose that $x_0, x_1, \ldots, x_n$ are roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 0, 1, \ldots, n$ the numbers w_i are defined by

$$w_i = \int_{-1}^{1} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx = \int_{-1}^{1} \ell_i(x)\, dx$$

Then

$$\int_{-1}^{1} f(x) dx = \sum_{i=0}^{n} w_i f(x_i),$$

where $f(x)$ is any polynomial of degree less or equal to $2n + 1$.

Do not!

!!!

When evaluating a quadrature rule

$$\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} w_i f(x_i).$$

do not generate the nodes and weights each time. Use a lookup table...

Example 1

GOAL Approximate $\int_1^{1.5} x^2 \ln(x)\, dx$ using Gaussian quadrature with $n = 1$.

SOLUTION As derived earlier, we want to use $\int_{-1}^{1} f(x)\, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$

- We also know from earlier, how to change the limits of integration:

$$\int_1^{1.5} f(x)\, dx = \int_{-1}^{1} f\left(\frac{(1.5-1)t + (1.5+1)}{2}\right) \frac{1.5-1}{2}\, dt$$

- Therefore, we are looking for the integral of

$$\frac{1}{4}\int_{-1}^{1} f\left(\frac{t+5}{4}\right) dt = \frac{1}{4}\int_{-1}^{1} \left(\frac{t+5}{4}\right)^2 \ln\left(\frac{t+5}{4}\right) dt$$

- Using Gaussian quadrature, our numerical integration becomes:

$$\frac{1}{4}\left[\left(\frac{-\frac{\sqrt{3}}{3}+5}{4}\right)^2 \ln\left(\frac{-\frac{\sqrt{3}}{3}+5}{4}\right) + \left(\frac{\frac{\sqrt{3}}{3}+5}{4}\right)^2 \ln\left(\frac{\frac{\sqrt{3}}{3}+5}{4}\right)\right] = 0.192268$$

Example 2

GOAL Approximate $\int_0^1 x^2 e^{-x}\, dx$ using Gaussian quadrature with $n = 1$.

SOLUTION We again want to convert our limits of integration to -1 to 1. Using the same process as the earlier example, we get:

$$\int_0^1 x^2 e^{-x} dx = \frac{1}{2}\int_{-1}^{1}\left(\frac{t+1}{2}\right)^2 e^{-(t+1)/2} dt.$$

Using the Gaussian roots we get:

$$\int_0^1 x^2 e^{-x} dx \approx \frac{1}{2}\left[\left(\frac{-\frac{\sqrt{3}}{3}+1}{2}\right)^2 e^{-(-\frac{\sqrt{3}}{3}+1)/2} + \left(\frac{\frac{\sqrt{3}}{3}+1}{2}\right)^2 e^{-(\frac{\sqrt{3}}{3}+1)/2}\right] = 0.15$$

Numerical Question

How does n point Gauss quadrature compare with n point Newton-Cotes...

Implementation Question

What about Composite Gauss quadrature?

Examples

with matlab...

Example

int_gauss.m: base routine for Gauss quadrature

Example

int_gauss_test.m: integrate $\int_0^5 xe^{-x}\,dx$ with

1. 1 subinterval, increasing number of nodes
2. 3 nodes, increases number of intervals

Result: GL quadrature with 1 subinterval and many nodes is more accurate when compared to GL quadrature with 3 nodes and many sub-intervals (for same number of function evaluations)

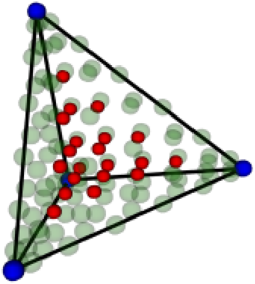
Example

int_compare_gauss_trapezoid_simpson.m: integrate $\int_0^5 xe^{-x}\,dx$ with

1. trapezoid
2. Simpson
3. Gauss

Result: Gauss quadrature is much more accurate for the same number of function evals.

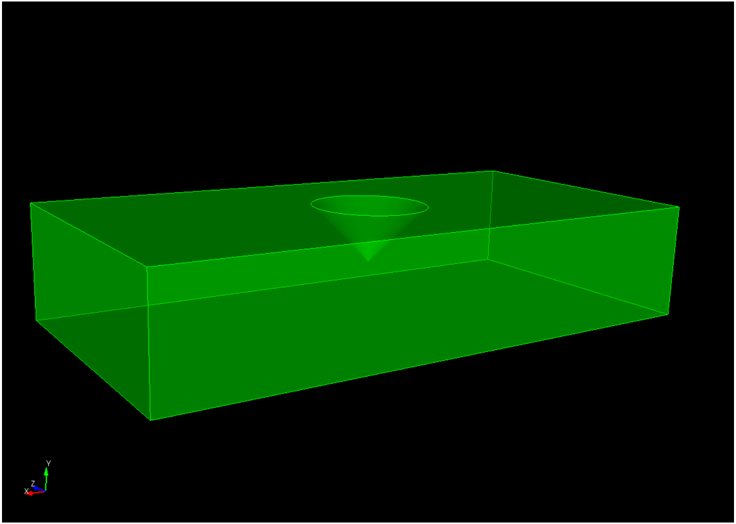
Something interesting...



- Gauss nodes in other shapes are not easy
- One approach: let electrostatics determine the (uneven) distribution

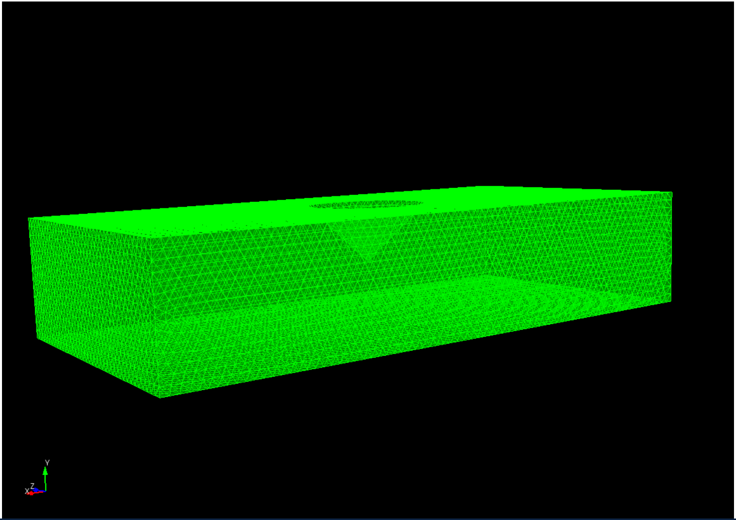
Quadrature

Consider quadrature over “interesting” 3D domain

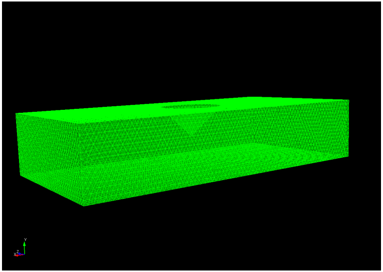


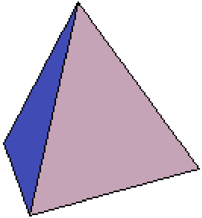
Quadrature

Consider quadrature over “interesting” 3D domain
- Break into ”subintervals” of 40K tetrahedrons, and integrate each tet



Quadrature





- 40K tetrahedrons.
- Need to integrate a function $f(x)$ over each tet Ω_i: $\int_{\Omega_i} f(x)\, dx$
- Needs quadrature
- Map the integration to a reference tetrahedron
- Perform Gauss Quadrature using $(n+1)(n+2)(n+3)/6$ quadrature points (where n is the 1-D number of points).
- Results in # of tetrahedrons $\times$ $n^3/6$ function evaluations