Numerical Methods 1

Physics 129AL

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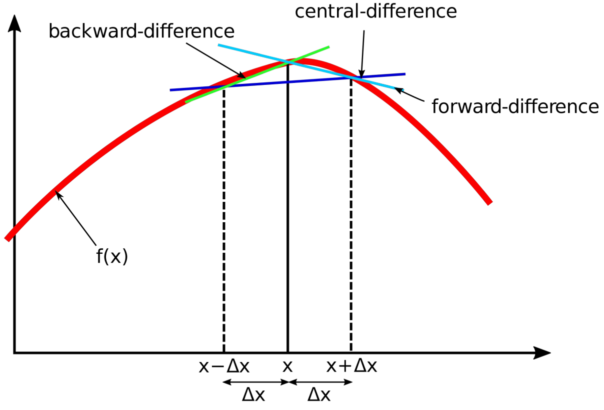
Numerical differentiation

The simplest method is to use finite difference,



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

$$f''(x) \approx \frac{\delta_h^2[f](x)}{h^2} = \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

https://en.wikipedia.org/wiki/Finite_difference

Numerical Integration

Numerical Integration (also called Quadrature)

$$I = \int_a^b f(x)dx$$

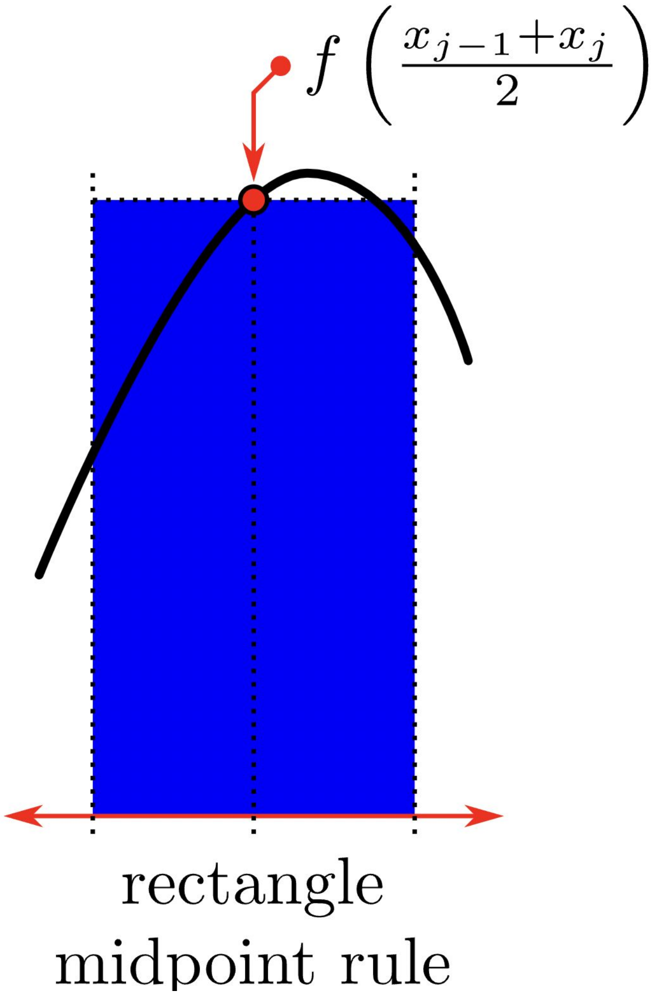
Special case of differential equation

$$\frac{dy}{dx} = f(x), \ \ y(a) = 0$$

Midpoint Rule

The midpoint rule M approximates the integral by the area of a rectangle whose base has length h and whose height is the value of f(x) at the midpoint (**order of 1/N^2**)

$$\int_{x_{j-1}}^{x_j} f(x)\,dx \approx f\left(\frac{x_{j-1}+x_j}{2}\right)\Delta x$$



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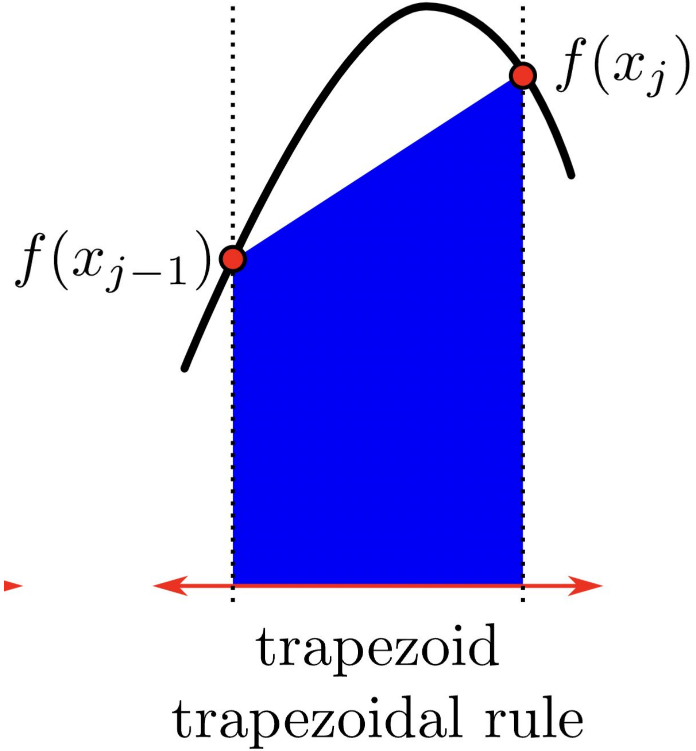
Trapezoidal Rule

The trapezoidal rule approximates the integral by the area of a trapezoid with base h and sides equal to the values of f(x) at the two end points. (**order of 1/N^2**)

$$\int_{x_{j-1}}^{x_j} f(x)\,dx \approx \frac{1}{2}\left[f(x_{j-1}) + f(x_j)\right]\Delta x$$

Trapezoid: $$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right]$$



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Example

The midpoint rule and the trapezoidal rule are both exact for constant functions and linear functions. **For higher order functions, which method is better?** Let's consider an example:

$$M = 1\left(\frac{1}{2}\right)^2 = \frac{1}{4}.$$

Midpoint rule Error: 1/12

$$\int_0^1 x^2\,dx = \frac{1}{3}.$$

$$T = 1\frac{0^2+1^2}{2} = \frac{1}{2}.$$

Trapezoidal rule Error: 1/6

Let the exact value of the integral be **I**

https://www.cs.usask.ca/~spiteri/M211/notes/chapter5.pdf

Example

If the error in T were exactly −2 times the error in M,

$$I - T = -2(I - M)$$

We can use it to approximate higher order integration. Let' give it a different name S,

$$S = \frac{2}{3}M + \frac{1}{3}T.$$

This is called Simpson's rule.

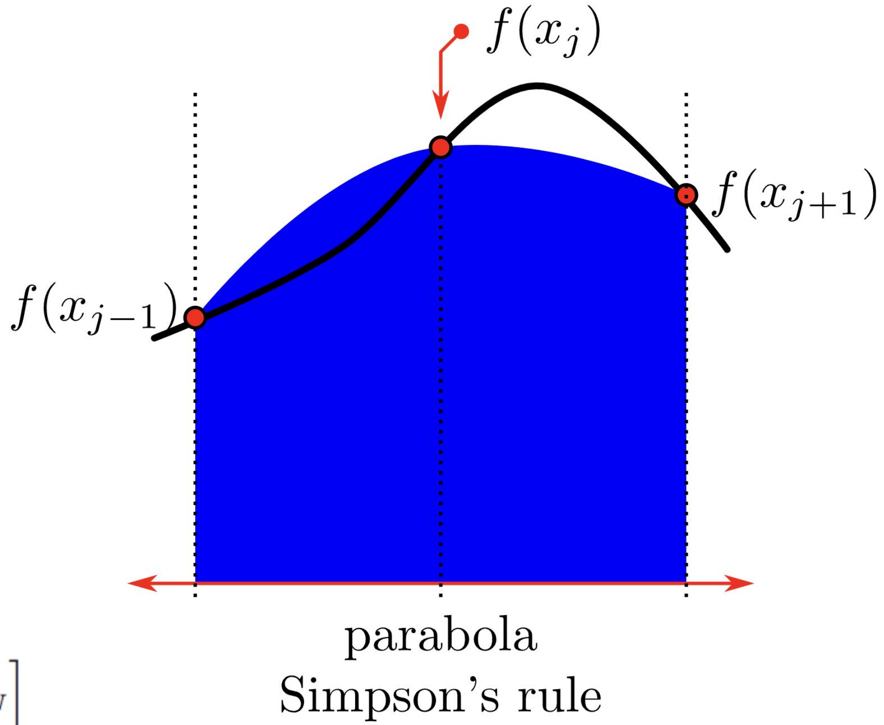
https://www.cs.usask.ca/~spiteri/M211/notes/chapter5.pdf

Simpson's rule

Classically, Simpson’s rule is derived by using a parabola to interpolate f(x) at the two endpoints, a and b, and the midpoint, (a+b)/2 and integrating the parabola exactly. (**order of N^4**)

$$\int_{x_{j-1}}^{x_{j+1}} f(x)\,dx \approx \frac{1}{3}\left[f(x_{j-1}) + 4f(x_j) + f(x_{j+1})\right]\Delta x$$

Simpson: $$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \cdots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right]$$



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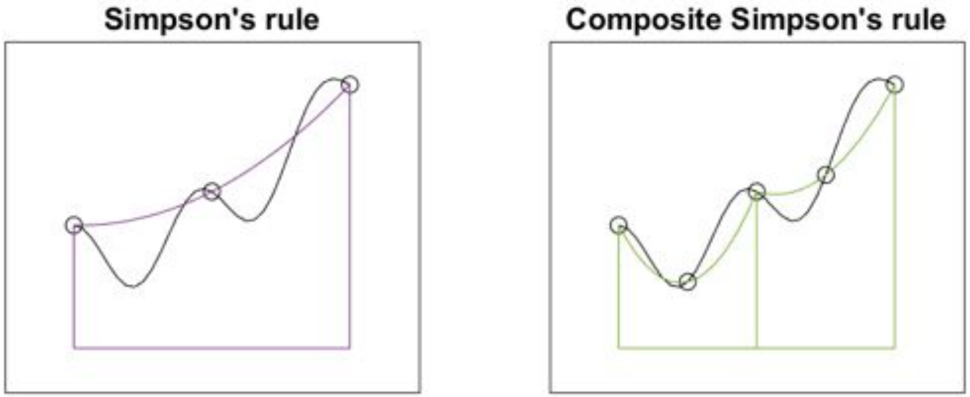
Richardson extrapolation

Can we in general combine lower accuracy terms to give higher accuracy terms by cancelling out the leading error? Let's take N to 2N and perform two simpson rule on two subintervals,



$$S_2 = \frac{h}{12}(f(a) + 4f(d) + 2f(c) + 4f(e) + f(b)).$$

https://blogs.mathworks.com/cleve/2016/05/23/modernization-of-numerical-integration-from-quad-to-integral/

Richardson extrapolation

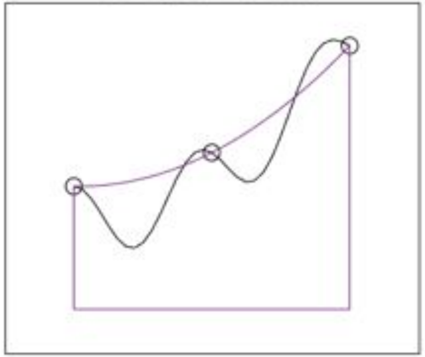
Since Simpson's rule is **order 4**, we can take N to 2N, and the error is expected to reduce by 2^4.

$$Q - S = 16(Q - S_2).$$

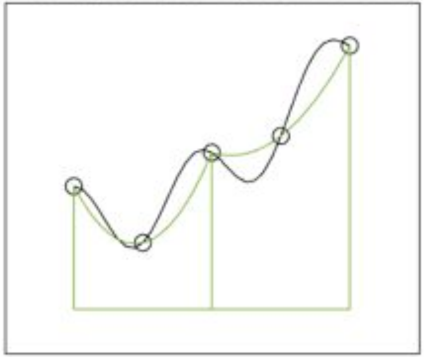
$$Q = S_2 + \frac{(S_2 - S)}{15}.$$

The result rule will be **order 6 in N**.

Simpson's rule



Composite Simpson's rule



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Richardson extrapolation and Romberg Integration

Richardson extrapolation involves taking two or more approximations of a quantity using different step sizes, and then combine these approximations to obtain a more accurate estimate. Following the same idea, we can cancel out the higher order errors by double the number of grid points: N, 2N, 4N, 8N…

Doubling N from I_1 to I_2,

$$I_1 + ch_1^2 = I_2 + ch_2^2,$$

$$I_2 - I_1 = ch_1^2 - ch_2^2 = 3ch_2^2,$$

$$\epsilon_2 = ch_2^2 = \tfrac{1}{3}(I_2 - I_1).$$

$$R_{i,1} = I_i\,,$$

$$R_{i,2} = I_i + \tfrac{1}{3}(I_i - I_{i-1}) = R_{i,1} + \tfrac{1}{3}(R_{i,1} - R_{i-1,1}).$$

$$\begin{array}{lllllll}
I_1 \equiv R_{1,1} & & & & & & \\
 & \searrow & & & & & \\
I_2 \equiv R_{2,1} & \to & R_{2,2} & & & & \\
 & \searrow & & \searrow & & & \\
I_3 \equiv R_{3,1} & \to & R_{3,2} & \to & R_{3,3} & & \\
 & \searrow & & \searrow & & \searrow & \\
I_4 \equiv R_{4,1} & \to & R_{4,2} & \to & R_{4,3} & \to & R_{4,4} \\
 & \searrow & & \searrow & & \searrow & & \searrow
\end{array}$$

Example

We will use *Romberg integration* to obtain a sixth-order accurate approximation to

$$\int_0^1 e^{-x^2}\,dx,$$

an integral that *cannot* be computed using the Fundamental Theorem of Calculus.

with $n = 1$ subintervals. Since $h = (b-a)/n = (1-0)/1 = 1$, we have

$$R_{1,1} = \frac{1}{2}[f(0) + f(1)] = 0.68393972058572,$$

which has an absolute error of 6.3×10^{-2}.

https://www.math.usm.edu/lambers/mat460/fall09/lecture29.pdf

Example

If we bisect the interval $[0, 1]$ into two subintervals of equal width, and approximate the area under e^{-x^2} using two trapezoids, then we are applying the Composite Trapezoidal Rule with $n = 2$ and $h = (1 - 0)/2 = 1/2$, which yields

$$R_{2,1} = \frac{0.5}{2}[f(0) + 2f(0.5) + f(1)] = 0.73137025182856,$$

which has an absolute error of 1.5×10^{-2}. As expected, the error is reduced by a factor of 4 when the step size is halved, since the error in the Composite Trapezoidal Rule is of $O(h^2)$.

Now, we can use Richardson Extrapolation to obtain a more accurate approximation,

$$R_{2,2} = R_{2,1} + \frac{R_{2,1} - R_{1,1}}{3} = 0.74718042890951,$$

which has an absolute error of 3.6×10^{-4}.

https://www.math.usm.edu/lambers/mat460/fall09/lecture29.pdf

Example

We can obtain a second approximation of fourth-order accuracy by using the Composite Trapezoidal Rule with $n = 4$ to obtain a third approximation of second-order accuracy. We set $h = (1-0)/4 = 1/4$, and then compute

$$R_{3,1} = \frac{0.25}{2}\left[f(0) + 2[f(0.25) + f(0.5) + f(0.75)] + f(1)\right] = 0.74298409780038,$$

which has an absolute error of 3.8×10^{-3}. Now, we can apply Richardson Extrapolation to $R_{2,1}$ and $R_{3,1}$ to obtain

$$R_{3,2} = R_{3,1} + \frac{R_{3,1} - R_{2,1}}{3} = 0.74685537979099,$$

which has an absolute error of 3.1×10^{-5}. This significant decrease in error from $R_{2,2}$ is to be expected, since both $R_{2,2}$ and $R_{3,2}$ have fourth-order accuracy, and $R_{3,2}$ is computed using half the step size of $R_{2,2}$.

https://www.math.usm.edu/lambers/mat460/fall09/lecture29.pdf

Example

Therefore, we can use Richardson Extrapolation with these two approximations to obtain a new approximation

$$R_{3,3} = R_{3,2} + \frac{R_{3,2} - R_{2,2}}{2^4 - 1} = 0.74683370984975,$$

which has an absolute error of 9.6×10^{-6}. Because $R_{3,3}$ is a linear combination of $R_{3,2}$ and $R_{2,2}$ in which the terms of order h^4 cancel, we can conclude that $R_{3,3}$ is of sixth-order accuracy. $\square$

Gaussian Quadratures

- an definite integral of f(x) can be projected to a new basis set g(x) with a give weight function W(x).

  - Those are then approximated by a sum of function values at specified points x_i multiplied by some weights w_i

    - In the case of Gauss-Legendre quadrature, the weighting function W=1.

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} W(x)g(x)\,dx$$

$$\int_{-1}^{1} W(x)g(x)\,dx \approx \sum_{i=1}^{n} w_i\,g(x_i)$$

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

Gaussian Quadratures

- This choice of quadrature weights wi and quadrature nodes xi is the unique choice that allows the quadrature rule to integrate degree 2n − 1 polynomials exactly. We solve the system of equations below for the case **n=2**,

$$\int_{-1}^{1} dx = 2 = w_1 + w_2$$

$$\int_{-1}^{1} x dx = 0 = w_1 x_1 + w_2 x_2$$

$$\int_{-1}^{1} x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

$$\int_{-1}^{1} x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3$$

$$x_1 = -x_2 = \frac{1}{\sqrt{3}}$$

$$w_1 = w_2 = 1$$

Gaussian Quadratures

- However, what if we want to have higher order, e.g. **n=3**? Solving the following system of equations is generally hard (since they are non-linear).

$$\int_{-1}^{1} dx = 2 = w_1 + w_2 + w_3$$

$$\int_{-1}^{1} x dx = 0 = w_1 x_1 + w_2 x_2 + w_3 x_3$$

$$\int_{-1}^{1} x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2$$

$$\int_{-1}^{1} x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3 + w_3 x_3^3$$

$$\int_{-1}^{1} x^4 dx = \frac{2}{5} = w_1 x_1^4 + w_2 x_2^4 + w_3 x_3^4$$

$$\int_{-1}^{1} x^5 dx = 0 = w_1 x_1^5 + w_2 x_2^5 + w_3 x_3^5$$

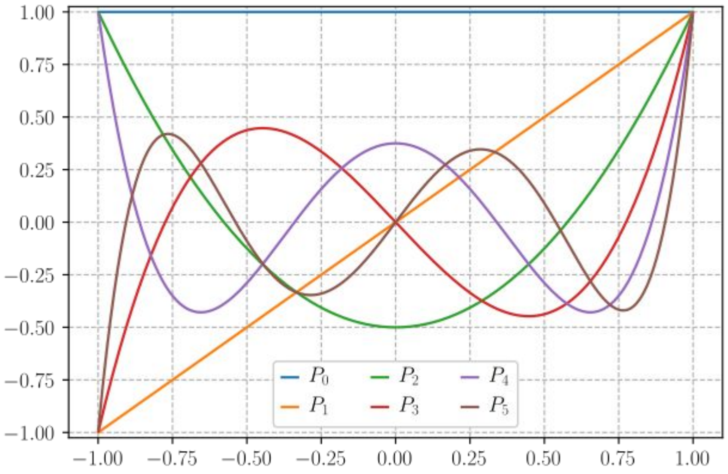
What can we do?

Gaussian Quadratures

- In fact, they are given exactly by the root of the **n-th Legendre polynomial**!

Legendre ODE $$(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0.$$

n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}\left(3x^2-1\right)$
3	$\frac{1}{2}\left(5x^3-3x\right)$
4	$\frac{1}{8}\left(35x^4-30x^2+3\right)$
5	$\frac{1}{8}\left(63x^5-70x^3+15x\right)$
6	$\frac{1}{16}\left(231x^6-315x^4+105x^2-5\right)$
7	$\frac{1}{16}\left(429x^7-693x^5+315x^3-35x\right)$
8	$\frac{1}{128}\left(6435x^8-12012x^6+6930x^4-1260x^2+35\right)$
9	$\frac{1}{128}\left(12155x^9-25740x^7+18018x^5-4620x^3+315x\right)$
10	$\frac{1}{256}\left(46189x^{10}-109395x^8+90090x^6-30030x^4+3465x^2-63\right)$



Gaussian Quadratures

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$$\int_{-1}^{1} dx = 2 = w_1 + w_2 + w_3$$
$$\int_{-1}^{1} x dx = 0 = w_1 x_1 + w_2 x_2 + w_3 x_3$$
$$\int_{-1}^{1} x^2 dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2$$
$$\int_{-1}^{1} x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3 + w_3 x_3^3$$
$$\int_{-1}^{1} x^4 dx = \frac{2}{5} = w_1 x_1^4 + w_2 x_2^4 + w_3 x_3^4$$
$$\int_{-1}^{1} x^5 dx = 0 = w_1 x_1^5 + w_2 x_2^5 + w_3 x_3^5$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x), \quad x_1 = -x_3 = \sqrt{\frac{3}{5}}, \quad x_2 = 0$$

And by plug in the roots into the system of equations, the weights are

$$w_i = \frac{2}{\left(1 - x_i^2\right)\left[P_n'(x_i)\right]^2}.$$

Gaussian Quadratures

For interval other than -1 to 1, we can perform a change of variable,

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

The values are numerically calculated,

Number of points, n	Points, x_i		Weights, w_i	
1	0		2	
2	$\pm\frac{1}{\sqrt{3}}$	±0.57735…	1	
3	0		$\frac{8}{9}$	0.888889…
	$\pm\sqrt{\frac{3}{5}}$	±0.774597…	$\frac{5}{9}$	0.555556…
4	$\pm\sqrt{\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.339981…	$\frac{18+\sqrt{30}}{36}$	0.652145…
	$\pm\sqrt{\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.861136…	$\frac{18-\sqrt{30}}{36}$	0.347855…
5	0		$\frac{128}{225}$	0.568889…
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$	±0.538469…	$\frac{322+13\sqrt{70}}{900}$	0.478629…
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	±0.90618…	$\frac{322-13\sqrt{70}}{900}$	0.236927…

Gaussian Quadratures

- Commonly used cases:

Rescale for other intervals

Gauss-Legendre:

$$W(x) = 1 \qquad -1 < x < 1$$

Gauss-Chebyshev:

$$W(x) = (1 - x^2)^{-1/2} \qquad -1 < x < 1$$

Gauss-Laguerre:

$$W(x) = x^\alpha e^{-x} \qquad 0 < x < \infty$$

Gauss-Hermite:

$$W(x) = e^{-x^2} \qquad -\infty < x < \infty$$

Gauss-Jacobi:

$$W(x) = (1 - x)^\alpha (1 + x)^\beta \qquad -1 < x < 1$$

Multidimensional Integrals

are HARD!

- Number of points scales as N^M, where M: # of dimensions
- Boundary can be complicated

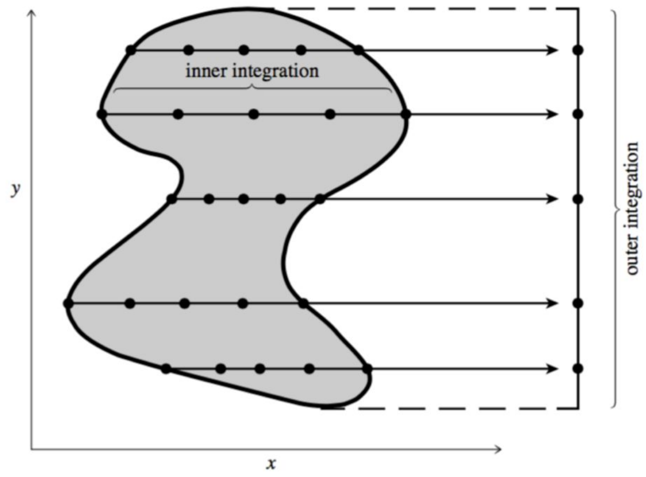
Can dimension be reduced?

$$\int_0^x dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_3} dt_2 \int_0^{t_2} f(t_1) dt_1$$
$$= \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t) dt$$

Multidimensional Integrals

If complicated boundary, low res, not strongly peaked integrand
→ Monte Carlo Integration (to be discussed later)

If boundary is simple and function is smooth
→ Repeated 1-D integrals



$$I = \int\int dx dy f(x, y)$$

$$H(x) = \int_{y_1}^{y_2} f(x, y) dy$$

$$I = \int_{x_1}^{x_2} H(x) dx$$

Best to use Gaussian Quadratures for high precision

Acknowledgement

The slides are partially developed or inspired by Professor Uros Seljak at UC Berkeley. For more information, please visit the github page.

A short story: When I was doing my undergraduate, I took his class (the exact same one, linked below).

https://phy151-ucb.github.io/seljak-phy151-fall-2018/#course-syllabus

Uros Seljak (Berkeley)