Numerical Integration (Quadrature)

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(based on material borrowed from Dennis Duke, Samir Al-Amer, David Kofke, Holistic Numerical Methods Institute)

Numerical Integration

Why do we need it?

- many integrals cannot be evaluated analytically
- even if you can, you might need to check your answer
- even if you can, numerical evaluation of the answer can be bothersome

Examples:

$$\int_0^\infty \frac{dx}{\sqrt{x}\cosh x} = 2\sqrt{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k}{\sqrt{2k+1}}$$

$$\int_a^b e^{-x^2}\,dx$$

Error function

An example of an integral that needs checking:

$$
\begin{aligned}
(3.15.7)\qquad \int_0^1 \frac{\ln(1+ay)\ln(1+by)}{1+cy}\,dy &= \frac{1}{c}\left\{\frac{1}{2}\ln^2\left(\frac{c-a}{c}\right)\ln(1+c) + \right.\\
&+ \frac{1}{2}\ln^2\left(\frac{c-b}{c}\right)\ln(1+c) - \frac{1}{2}\ln^2\left(\frac{a}{b}\right)\ln(1+b) +\\
&+ \frac{1}{2}\ln^2\left(\frac{a-c}{b-c}\right)\ln\left(\frac{1+b}{1+c}\right) + \ln\left(\frac{c-a}{c}\right)\left[\mathrm{Li}_2\left(\frac{a}{a-c}\right) - \mathrm{Li}_2\left(a\frac{1+c}{a-c}\right)\right] +\\
&+ \ln\left(\frac{c-b}{c}\right)\left[\mathrm{Li}_2\left(\frac{b}{b-c}\right) - \mathrm{Li}_2\left(b\frac{1+c}{b-c}\right)\right] + S_{1,2}\left(a\frac{1+c}{a-c}\right) -\\
&- S_{1,2}\left(\frac{a}{a-c}\right) + S_{1,2}\left(b\frac{1+c}{b-c}\right) - S_{1,2}\left(\frac{b}{b-c}\right) - S_{1,2}\left(\frac{a-b}{a}\right) +\\
&+ S_{1,2}\left(\frac{a-b}{a(1+b)}\right) - S_{1,2}\left(\frac{(a-b)(1+c)}{(a-c)(1+b)}\right) + S_{1,2}\left(\frac{a-b}{a-c}\right) +\\
&+ \ln\left(\frac{a}{b}\right)\left[\mathrm{Li}_2\left(\frac{a-b}{a}\right) - \mathrm{Li}_2\left(\frac{a-b}{a(1+b)}\right)\right] +\\
&\left. + \ln\left(\frac{a-c}{b-c}\right)\left[\mathrm{Li}_2\left(\frac{(a-b)(1+c)}{(a-c)(1+b)}\right) - \mathrm{Li}_2\left(\frac{a-b}{a-c}\right)\right]\right\}
\end{aligned}
$$

$$
\mathrm{Li}_2(y) = -\int_0^1 \frac{\ln(1-xy)}{x}\,dx = -\int_0^y \frac{\ln(1-x)}{x}\,dx
$$

$$
S_{1,2}(y) = \frac{1}{2}\int_0^1 \frac{\ln^2(1-xy)}{x}\,dx
$$

Possible Issues

the integrand is some sort of table of numbers

- regularly spaced
- irregularly spaced
- contaminated with noise *(experimental data)*

the integrand is computable everywhere in the range of integration, but there may be

- infinite range of integration
- local discontinuities

considerations

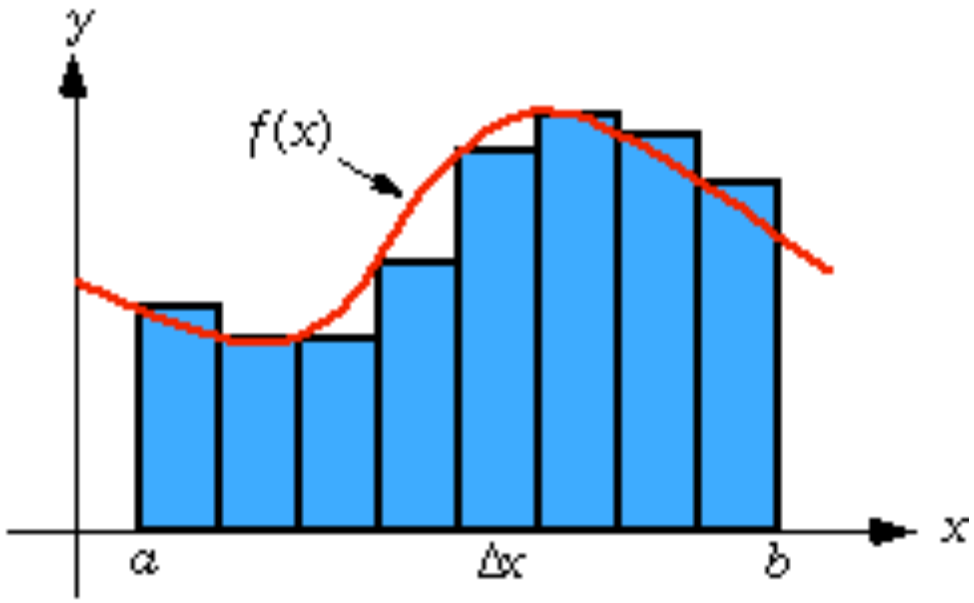
- time to compute the integral
- estimate of the error due to
  - truncation
  - round-off
  - noise in tabulated values

Integral as Riemann sum

• In the differential limit, an integral is equivalent to a summation operation:

$$\int_a^b f(x)dx = \lim_{n\to\infty} \sum_{i=0}^{i=n} f(x_i)\Delta x \approx \sum_{i=0}^{N-1} f(x_i)\Delta x$$

• Approximate methods for determining integrals are mostly based on idea of area between integrand and axis.



Let's try a simple example

n	intervals	dx	error
1	2	0.785398	-0.340759
2	4	0.392699	-0.183465
3	8	0.196350	-0.094960
4	16	0.098175	-0.048284
5	32	0.049087	-0.024343
6	64	0.024544	-0.012222
7	128	0.012272	-0.006123
8	256	0.006136	-0.003065
9	512	0.003068	-0.001533
10	1024	0.001534	-0.000767

Analytically

$$\int_0^{\pi/2} \cos x\, dx = \sin x \Big|_0^{\pi/2} = 1$$

Note that the error is decreasing by a factor 2, just like our discretization interval *dx*.

Question: Why is the error = I(exact) - I(calc) negative?

Instead of having the top of the rectangle hit the left (or right) edge we could also have it hit the function at the midpoint of each interval:

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

n	intervals	dx	error
1	2	0.785398	-0.026172153
2	4	0.392699	-0.006454543
3	8	0.196350	-0.001608189
4	16	0.098175	-0.000401708
5	32	0.049087	-0.000100406
6	64	0.024544	-0.000025100
7	128	0.012272	-0.000006275
8	256	0.006136	-0.000001569
9	512	0.003068	-0.000000392
10	1024	0.001534	-0.000000098

now the error is falling **by a factor 4** with each halving of the interval *dx*.

Note that the lines at the top of the rectangles can have any slope whatsoever and we will always get the same answer.

Question: Why is the error smaller?

Question: Why is the error smaller?

Answer:

• One reason is that in the mid-point rule, the maximum distance over which we "extrapolate" our knowledge of f(x) is halved.

• Different integration schemes result from what we think the function is doing between evaluation points.

• Link between interpolation and numerical integration

Orientation

- Newton-Cotes Methods

  Use intepolating polynomials. Trapezoid, Simpson's 1/3 and 3/8 rules, Bode's are special cases of 1st, 2nd, 3rd and 4th order polynomials are used, respectively

- Romberg Integration (Richardson Extrapolation)

  use knowledge of error estimates to build a recursive higher order scheme

- Gauss Quadrature

  Like Newton-Cotes, but instead of a regular grid, choose a set that lets you get higher order accuracy

- Monte Carlo Integration

  Use randomly selected grid points. Useful for higher dimensional integrals (d>4)

Newton-Cotes Methods

- In Newton-Cotes Methods, the function is approximated by a polynomial of order *n*
- To do this, we use ideas learnt from interpolation
- Computing the integral of a polynomial is easy.

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x + \ldots + a_n x^n\right)dx$$

we approximate the function *f(x)* in the interval *[a,b]* as:

$$f(x) \approx a_0 + a_1 x + \ldots + a_n x^n$$

interpolation

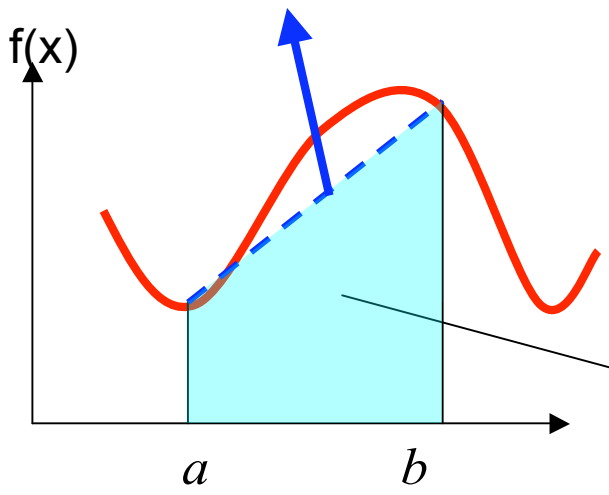
$$\int_a^b f(x)dx \approx a_0(b-a) + a_1 \frac{(b^2 - a^2)}{2} + \ldots + a_n \frac{(b^{n+1} - a^{n+1})}{n+1}$$

Newton-Cotes Methods

Trapezoid Method (First Order Polynomial are used)

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1 x)dx$$

$$f(a) + \frac{f(b)-f(a)}{b-a}(x-a)$$



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

$$I \approx \int_a^b \left(f(a) + \frac{f(b)-f(a)}{b-a}(x-a) \right) dx$$

$$= \left(f(a) - a\frac{f(b)-f(a)}{b-a} \right) x \Big|_a^b + \frac{f(b)-f(a)}{b-a}\frac{x^2}{2}\Big|_a^b$$

$$= (b-a)\frac{f(b)+f(a)}{2}$$

Multi-step Trapezoid Method

If the interval is divided into n segments(not necessarily equal)

$$a = x_0 \le x_1 \le x_2 \le \ldots \le x_n = b$$

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

Special Case (Equally spaced base points)

$$x_{i+1} - x_i = h \quad \text{for all} \quad i$$

$$\int_a^b f(x)dx \approx h\left[\frac{1}{2}\left[f(x_0) + f(x_n)\right] + \sum_{i=1}^{n-1} f(x_i)\right]$$

Multi-step Trapezoid Method

n	intervals	dx	error
1	2	0.78539816	0.05194055
2	4	0.39269908	0.01288420
3	8	0.19634954	0.00321483
4	16	0.09817477	0.00080332
5	32	0.04908739	0.00020081
6	64	0.02454369	0.00005020
7	128	0.01227185	0.00001255
8	256	0.00613592	0.00000314
9	512	0.00306796	0.00000078
10	1024	0.00153398	0.00000020

$$\int_0^{\pi/2} \cos x\,dx = \sin x\Big|_0^{\pi/2} = 1$$

Now the error is again decreasing by a factor 4, so like dx^2.

In fact, it can be shown that:

$$|Error| \le \frac{b-a}{12}\, h^2 \max_{x\in[a,b]} |f''(x)|$$

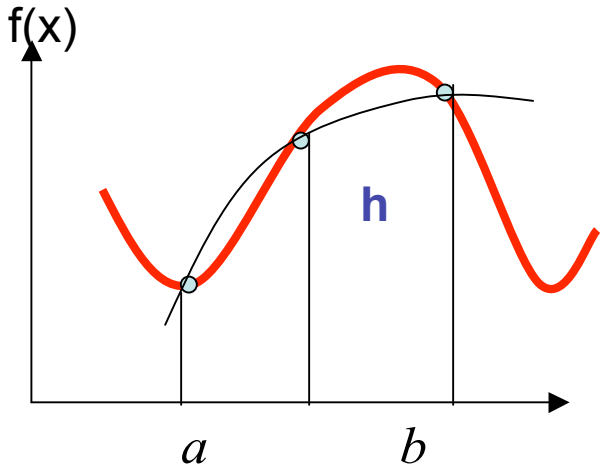
Newton-Cotes Methods

Simpson 1/3 Rule

Second Order Polynomial are used

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

h=(b-a)/2

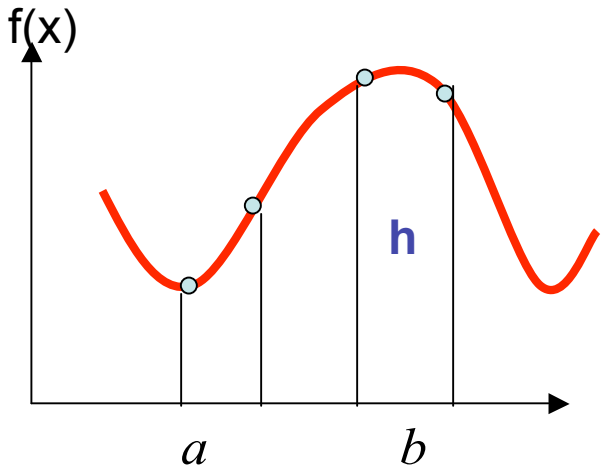


Simpson 3/8 Rule

Third Order Polynomial are used,

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)dx$$

h=(b-a)/3



Newton-Cotes Methods

Closed Newton–Cotes Formulas

Degree	Common name	Formula	Error term
1	Trapezoid rule	$\frac{h}{2}(f_0 + f_1)$	$-\frac{h^3}{12} f^{(2)}(\xi)$
2	Simpson's rule	$\frac{h}{3}(f_0 + 4f_1 + f_2)$	$-\frac{h^5}{90} f^{(4)}(\xi)$
3	Simpson's 3/8 rule	$\frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$	$-\frac{3h^5}{80} f^{(4)}(\xi)$
4	Boole's rule, or Bode's Rule [sic]	$\frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$	$-\frac{8h^7}{945} f^{(6)}(\xi)$

These are called “closed” because we use function evaluations at the end-points of the interval. There are “open” formulae which don’t evalute *f(a)* and *f(b)*, but we won’t discuss them here.

wikipedia.org

Romberg Integration

- Trapezoid formula with an interval *h* gives error of the order $O(h^2)$

- Can we combine two Trapezoid estimates with intervals *2h* and *h* to get a better estimate?

- For a multistep trapezoidal rule, the error is:

$$E_t = \frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

where $\xi_i \in [\, a+(i-1)h,\ a+ih \,]$

- Think of $\frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$ as an approximate average value of *f"(x) in [a,b]*. Then,

$$E_t \cong \frac{C}{n^2}$$

Romberg Integration

How good is this approximation?

Consider

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

Vertical distance covered by a rocket between 8 to 30 seconds

n	Value	E_t
1	11868	807
2	11266	205
3	11153	91.4
4	11113	51.5
5	11094	33.0
6	11084	22.9
7	11078	16.8
8	11074	12.9

Exact value x=11061 meters

Romberg Integration

The true error gets approximately quartered as the number of segments is doubled. This information is used to get a better approximation of the integral, and is the basis of Romberg Integration (or Richardson's extrapolation).

$$E_t \cong \frac{C}{n^2}$$ where C is an *approximately constant*

If I_{true} = true value and I_n= approx. value of the integral

$$I_{true} \approx I_n + E_t$$

$$E_t(n) \approx C/n^2 \approx I_{true} - I_n$$

$$E_t(2n) \approx C/4n^2 \approx I_{true} - I_{2n}$$

Therefore, eliminate C/n^2 between these two equations

$$I_{true} \cong I_{true,est} = I_{2n} + \frac{I_{2n} - I_n}{3}$$

Note: What we calculate is still an approximation for I_{true}

Example

The vertical distance covered by a rocket from 8 to 30 seconds is given by

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

Exact value=11061 meters

1. Use Richardson's rule to find the distance covered (use table for multistep trapezoidal rule).
2. Find the true error, E_t for part (1).

n	Value	E_t	RelErr
1	11868	807	7.296
2	11266	205	1.854
3	11153	91.4	0.8265
4	11113	51.5	0.4655
5	11094	33.0	0.2981
6	11084	22.9	0.2070
7	11078	16.8	0.1521
8	11074	12.9	0.1165

Multistep trapezoidal rule

Solution

$$I_2 = 11266m$$

$$I_4 = 11113m$$

Using Richardson's extrapolation formula for Trapezoidal rule, choosing n=2

$$I_{true} \cong I_{2n} + \frac{I_{2n} - I_n}{3}$$

= 11062 m ($I_{true,est}$)

$E_t = I_{exact} - I_{true,est} = -1\ m$

$$|\in_t| = \left|\frac{11061 - 11062}{11061}\right| \times 100$$

Solution

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

n	Trapezoidal Rule	e_t for Trapezoidal Rule	Richardson's Extrapolation	e_t for Richardson's Extrapolation
1	11868	7.296	--	--
2	11266	1.854	11065	0.03616
4	11113	0.4655	11062	0.009041
8	11074	0.1165	11061	0.0000

Usually much better estimates

Romberg Integration: Successive Refinement

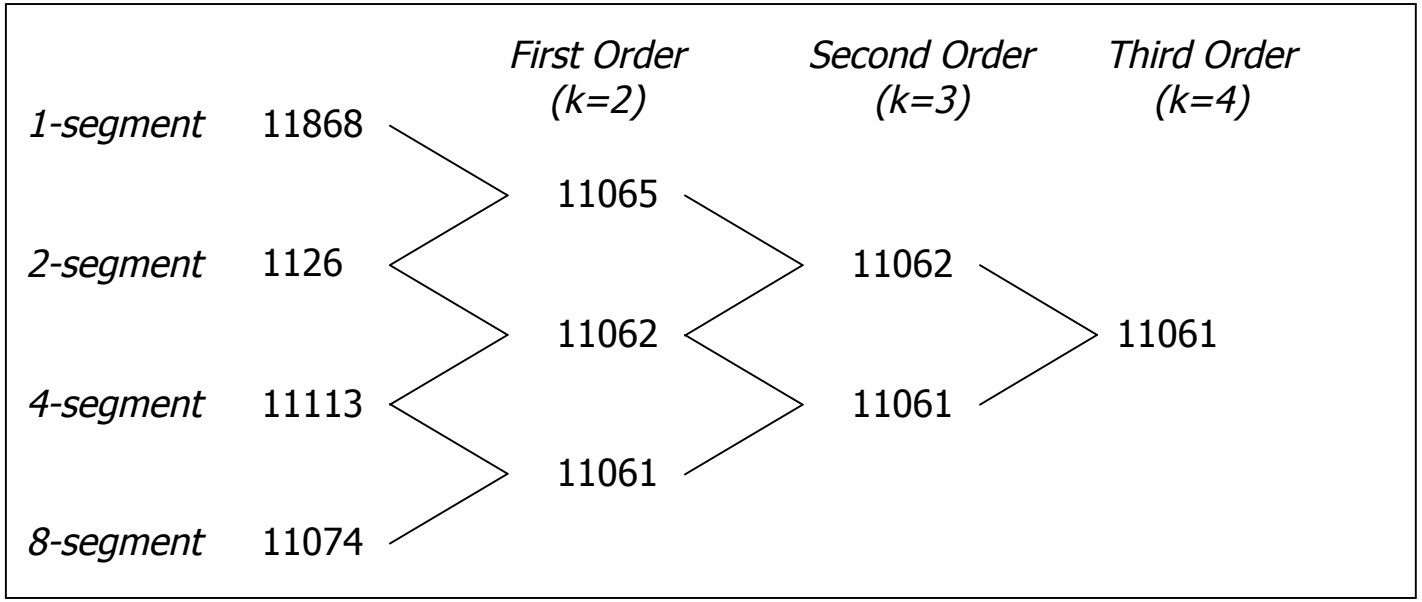
A general expression for Romberg integration can be written as

$$I_{2n}^{(k)} = \frac{4^k I_{2n}^{(k-1)} - I_n^{(k-1)}}{4^{k-1} - 1}, k \geq 2$$

- *The index k represents the order of extrapolation.*
- *$I_n^{(1)}$ represents the values obtained from the regular Trapezoidal rule with n intervals.*
- *k=2 represents values obtained using the true estimate as $O(h^2)$.*
- *$I_n^{(k)}$ has an error of the order $1/n^{2k}$.*

Romberg Integration: Successive Iteration

For our particular example:



Questions from last class:

1. What is the error in Romberg integration?

$$I_{true} \cong I_{true,est} = I_{2n} + \frac{I_{2n} - I_n}{3}$$

O(1/n^4)

$$E_t \cong \frac{C_1}{n^2} + \frac{C_2}{n^4} + \frac{C_3}{n^6} \ldots$$

Over here identical to Simpson's rule.

In fact this is how Numerical Recipes (Press et al.) implements the Simpson's rule

Successive iterations:

$$I_{2n}^{(k)} = \frac{4^k I_{2n}^{(k-1)} - I_n^{(k-1)}}{4^{k-1} - 1}, k \geq 2$$

This has an error of the order 1/n^{2k}.

Questions from last class:

2. Is Romberg better than Simpson's?

Successive iterations:

$$I_{2n}^{(k)} = \frac{4^k I_{2n}^{(k-1)} - I_n^{(k-1)}}{4^{k-1} - 1}, k \geq 2$$

This has an error of the order $1/n^{2k}$.

So usually, yes!

To evaluate an integral to the same degree of accuracy, you need fewer function evaluations with Romberg.

Numerical Recipes:

$$\int_0^2 x^4 \log(x + \sqrt{x^2 + 1})dx$$

Simpson's rule makes 8 times as many function calls

Romberg Integration

Questions:

1. Do I have to use I_n and I_{2n}?

2. Is this true only for the trapezoidal rule?

Romberg Integration

Questions:

1. Do I have to use I_n and I_{2n}?

2. Is this true only for the trapezoidal rule?

No!

But you have to derive new relationships in lieu of:

$$I_{2n}^{(k)} = \frac{4^k I_{2n}^{(k-1)} - I_n^{(k-1)}}{4^{k-1} - 1}, k \geq 2$$

But note that it may destroy “recursive structure” used in the expression above to minimize function calls.

Gauss Quadrature

Motivation

Multistep Trapezoid Method

$$\int_a^b f(x)dx = h\left[\sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}\left(f(x_0) + f(x_n)\right)\right]$$

It can be expressed as

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

$$where \;\; c_i = \begin{cases} h & i = 1,2,\ldots,n-1 \\ 0.5\,h & i = 0 \;\; and \;\; n \end{cases}$$

Gauss Quadrature

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

$$c_i : Weights \qquad x_i : Nodes$$

Problem

How do we select ***c_i and x_i*** so that the formula gives a better (higher order) approximation of the integral?

Approximate function with Polynomial

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx$$

where $P_n(x)$ is a polynomial that interpolates f(x) at the nodes $x_0, x_1, \ldots, x_n$

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \int_a^b \left(\sum_{i=0}^{n} \ell_i(x) f(x_i) \right) dx$$

$$\Rightarrow \int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i \; f(x_i) \quad \textit{where} \;\; c_i = \int_a^b \ell_i(x)\,dx$$

- If the points x_i are chosen on a uniform grid, this is exactly Newton-Cotes

Newton-Cotes

For a uniform grid $\{ x_i \}$ $P_n(x)$ is exact if $f(x)$ is a polynomial $d(n)$

Gaussian Quadrature

Choose the $n+1$ grid points $\{ x_i \}$ so that the polynomial
$P_n(x)$ is exact if f(x) is a polynomial d(2n+1)

How do we get nodes and weights

Example:

Can we select nodes and weights so that a (n+1)=2 nodes allow us to write a formula that is exact for polynomials of degree (2n+1) = 3?

$$\int_{-1}^{1} f(x)\,dx = c_0 f(x_0) + c_1 f(x_1)$$

Brute Force:

Set up equations for all polynomials d(0) to d(2n+1) and solve for c_i and x_i

$$f(x) = 1; \quad c_0 + c_1 = \int_{-1}^{1} 1\, dx = 2$$

$$f(x) = x; \quad c_0 x_0 + c_1 x_1 = \int_{-1}^{1} x\, dx = 0$$

$$f(x) = x^2; \quad c_0 {x_0}^2 + c_1 {x_1}^2 = \int_{-1}^{1} x^2\, dx = 2/3$$

$$f(x) = x^3; \quad c_0 {x_0}^3 + c_1 {x_1}^3 = \int_{-1}^{1} x^3\, dx = 2$$

Solve simultaneously, get

$$c_0 = c_1 = 1$$

$$x_0 = -1/\sqrt{3}; x_1 = 1/\sqrt{3}$$

Nodes and weights for larger n:

c_i

Number of points, n	Points, x_i	Weights, w_i
1	0	2
2	$\pm\sqrt{1/3}$	1
3	0	$8/9$
	$\pm\sqrt{3/5}$	$5/9$
4	$\pm\sqrt{\left(3-2\sqrt{6/5}\right)/7}$	$\frac{18+\sqrt{30}}{36}$
	$\pm\sqrt{\left(3+2\sqrt{6/5}\right)/7}$	$\frac{18-\sqrt{30}}{36}$
5	0	$128/225$
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{10/7}}$	$\frac{322+13\sqrt{70}}{900}$
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{10/7}}$	$\frac{322-13\sqrt{70}}{900}$

wikipedia.org

What is my limits are not [-1,1]?

For a range of integration other than *[-1,1]*, change of variables

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

$$= \frac{b-a}{2}\sum_{i=1}^{n} c_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Example

$$\int_0^1 e^{-x^2}\,dx = \frac{1}{2}\int_{-1}^{1} e^{-(.5t+.5)^2}\,dt$$

$$= \frac{1}{2}\left[e^{-\left(-0.5\sqrt{\frac{1}{3}}+.5\right)^2} + e^{-\left(0.5\sqrt{\frac{1}{3}}+.5\right)^2} \right]$$

2 points

Advantages/Disadvantages

1. For functions that are smooth or approximately polynomial beats Newton-Cotes in accuracy.

$$\operatorname{erf}(1) = \frac{2}{\pi}\int_0^1 e^{-x^2}\,dx$$

with n=3, get 5 correct significant places

2. Not easy to get error bounds (need to know derivative f^{2n+2}).

3. Unlike Romberg Integration, we cannot successively refine (Gauss-Konrad tries to overcome that.)

Gauss Quadrature: Generalization

What we just looked at was a special case of:

$$\int_a^b w(x) f(x)\, dx = \sum_{i=1}^{n} c_i f(x_i)$$

with w(x) = 1. This is called Gauss-Legendre.

There are other forms of Gauss Quadrature (not only Gauss-Legendre) which are useful, when:

1. there are discontinuties,
2. range of integration is not finite,
3. when the weight w(x) can help the function “look” more polynomial
4. Etc.

Generalization

The fundamental theorem of Gaussian quadrature states that the optimal nodes x_i of the n-point Gaussian quadrature formulas are precisely the roots of the orthogonal polynomial for the same interval and weighting function.

Generalization

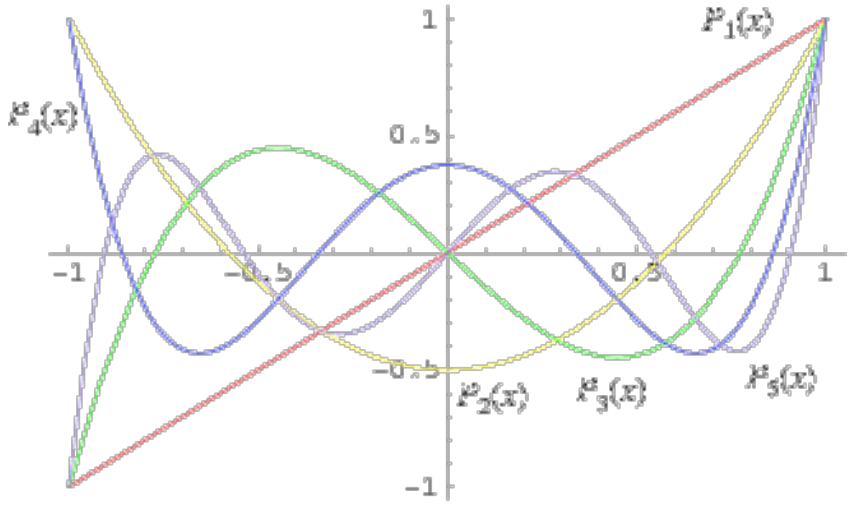
$$\int_a^b w(x) f(x)\, dx = \sum_{i=1}^{n} c_i f(x_i)$$

Interval	ω(x)	Orthogonal polynomials	A & S	For more information, see ...
[−1, 1]	1	Legendre polynomials	25.4.29	Section *Rules for the basic problem*, above
(−1, 1)	$(1-x)^{\alpha}(1+x)^{\beta}, \quad \alpha, \beta > -1$	Jacobi polynomials	25.4.33 (β = 0)	
(−1, 1)	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (first kind)	25.4.38	Chebyshev–Gauss quadrature
[−1, 1]	$\sqrt{1-x^2}$	Chebyshev polynomials (second kind)	25.4.40	Chebyshev–Gauss quadrature
[0, ∞)	e^{-x}	Laguerre polynomials	25.4.45	Gauss–Laguerre quadrature
(−∞, ∞)	e^{-x^2}	Hermite polynomials	25.4.46	Gauss–Hermite quadrature

wikipedia

Gauss-Legendre

Number of points, n	Points, x_i	Weights, w_i
1	0	2
2	$\pm\sqrt{1/3}$	1
3	0	$8/9$
	$\pm\sqrt{3/5}$	$5/9$
4	$\pm\sqrt{\left(3-2\sqrt{6/5}\right)/7}$	$\frac{18+\sqrt{30}}{36}$
	$\pm\sqrt{\left(3+2\sqrt{6/5}\right)/7}$	$\frac{18-\sqrt{30}}{36}$
5	0	$128/225$
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{10/7}}$	$\frac{322+13\sqrt{70}}{900}$
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{10/7}}$	$\frac{322-13\sqrt{70}}{900}$



All we do are look for zeros of $P_n(x)$ in *[-1,1].* These are our x_is.

The c_is can be obtained from

$$c_i = \frac{2}{(1-x_i^2)(P_n'(x_i))^2}$$

Generalization

In practice,

1. Gauss-Legendre is the most widely used Gauss quadrature formula.

2. We look at the limits and the weighting function *w(x)* for the integral we want to evaluate and decide what quadrature formula might be best.

3. We don't calculate the nodes and weights ourselves. Instead, we look them up for a give *n*, and simply carry out the weighted sum.

   http://www.efunda.com/math/num_integration/num_int_gauss.cfm

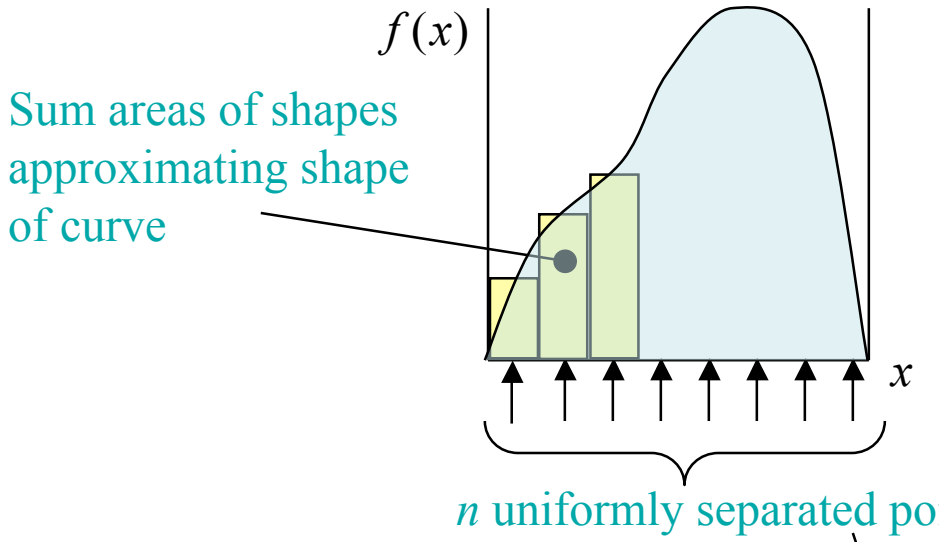
4. Note that this may require a change of variables.

Monte Carlo Integration

Adapting notes from David Kofke's
Molecular Simulation class.

One-Dimensional Integrals

- Methodical approaches
  - *trapezoid rule, Simpson's rule, Gauss quadrature*



Evaluating the general integral $I = \int_a^b f(x)dx$

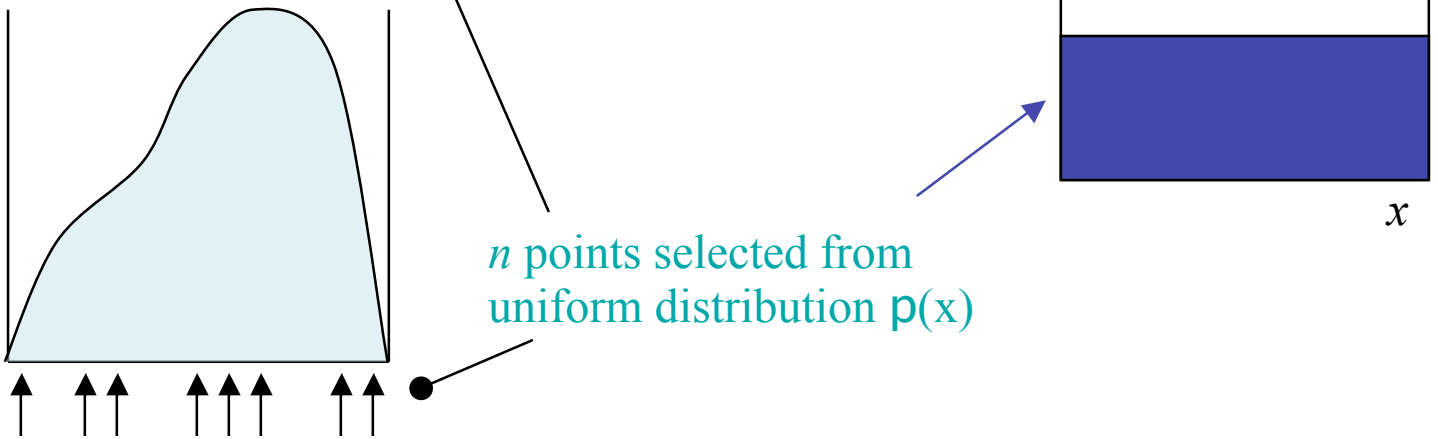
- Quadrature formula

$$I \approx \Delta x \sum_{i=1}^{n} f(x_i) = \frac{b-a}{n} \sum_{i=1}^{n} f(x_i)$$

Monte Carlo Integration

- Stochastic approach
- Same quadrature formula, different selection of points

$$I \approx \frac{b-a}{n} \sum_{i=1}^{n} f(x_i)$$



- http://www.eng.buffalo.edu/~kofke/ce530/Applets/applets.html

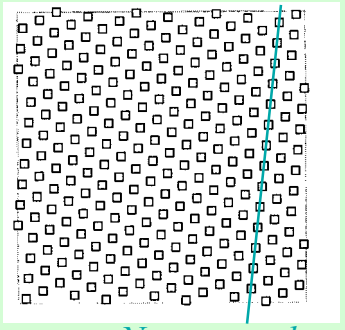
Random Number Generation

- Random number generators
  - subroutines that provide a new random deviate with each call
  - basic generators give value on (0,1) with uniform probability
  - uses a deterministic algorithm (of course)
    - *usually involves multiplication and truncation of leading bits of a number*

$$X_{n+1} = (aX_n + c) \bmod m$$ *linear congruential sequence*

- Returns set of numbers that meet many statistical measures of randomness
  - histogram is uniform
  - no systematic correlation of deviates
    - *no idea what next value will be from knowledge of present value (without knowing generation algorithm)*
    - *but eventually, the series must end up repeating*
- Some famous failures
  - be careful to use a good quality generator

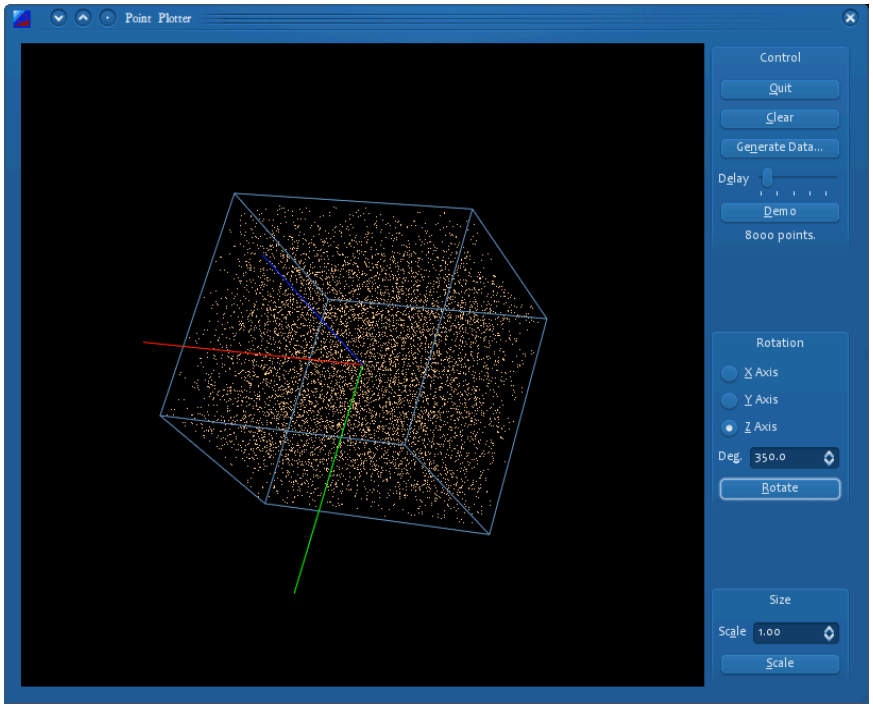
Plot of successive deviates (X_n, X_{n+1})

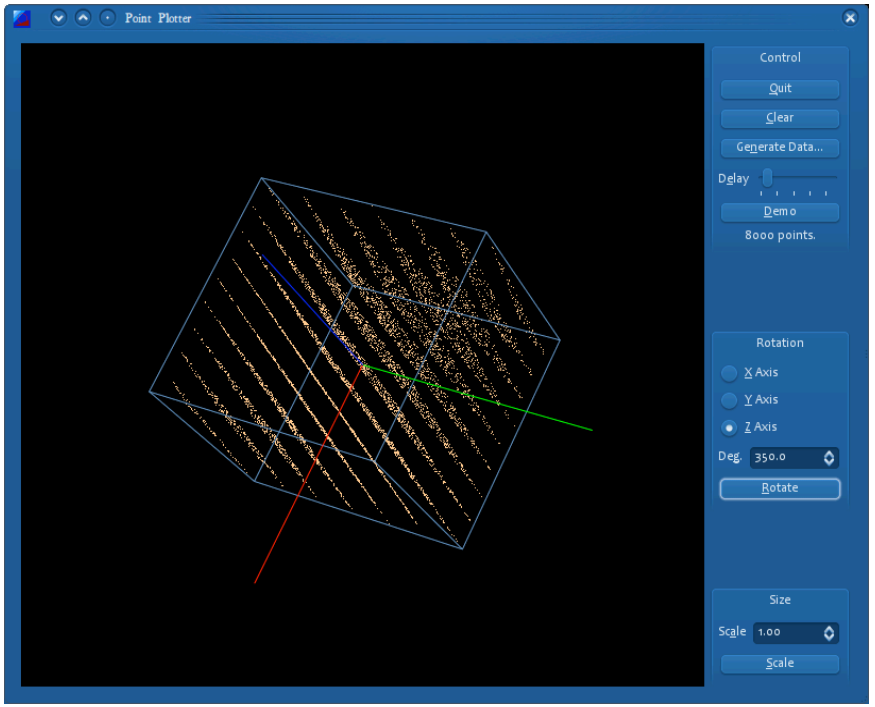


Not so random!

Random Number Generation

- RANDU
  - Linear congruential sequence developed in the 1960s at IBM





Not so random!

http://www.purinchu.net/wp/2009/02/06/the-randu-pseudo-random-number-generator/

Errors in Random vs. Methodical Sampling

- Comparison of errors
  - methodical approach
  - Monte Carlo integration

for example (Simpson's rule)

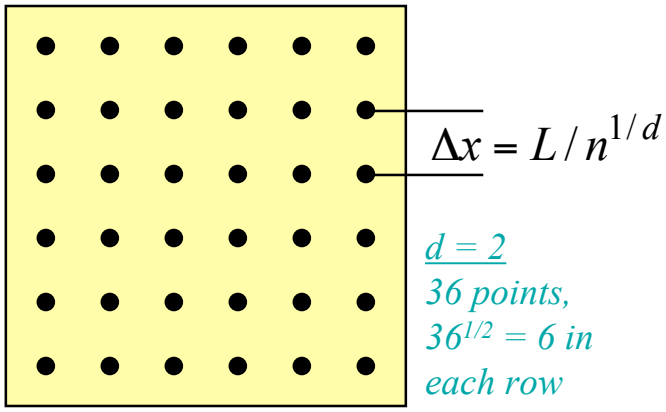
$$\delta I \propto \Delta x^2 \propto n^{-2}$$

$$\delta I \propto n^{-1/2}$$

- MC error vanishes much more slowly for increasing *n*
- For one-dimensional integrals, MC offers no advantage
- This conclusion changes as the dimension *d* of the integral increases
  - *methodical approach* $\delta I \propto n^{-2/d}$
  - *MC integration* $\delta I \propto n^{-1/2}$

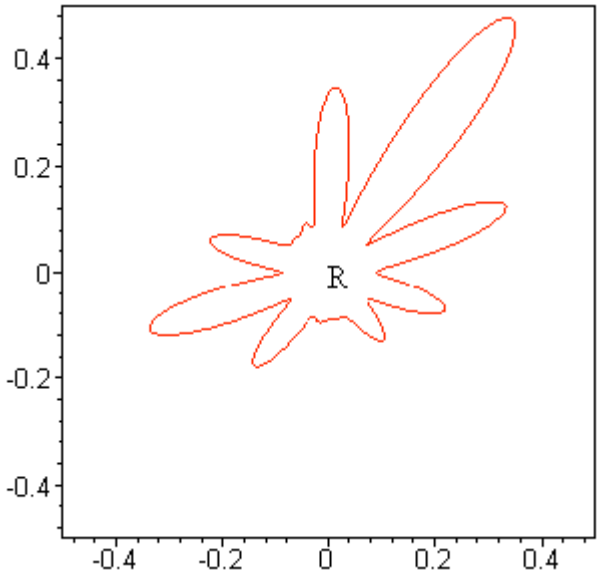
independent of dimension!

- MC "wins" at about *d* = *4*



Shape of High-Dimensional Regions

- Two (and higher) dimensional shapes can be complex
- How to construct and weight points in a grid that covers the region *R*?

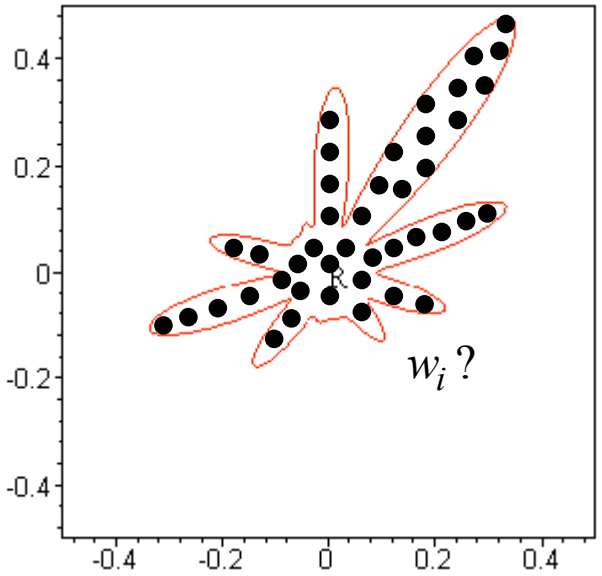


Example: mean-square distance from origin

$$\left\langle r^2 \right\rangle = \frac{\iint_R (x^2 + y^2)\,dxdy}{\iint_R dxdy}$$

Shape of High-Dimensional Regions

- Two (and higher) dimensional shapes can be complex
- How to construct and weight points in a grid that covers the region *R*?
  - *hard to formulate a methodical algorithm in a complex boundary*
  - *usually do not have analytic expression for position of boundary*
  - *complexity of shape can increase unimaginably as dimension of integral grows*



Example: mean-square distance from origin

$$\left\langle r^2 \right\rangle = \frac{\iint_R (x^2 + y^2)\,dxdy}{\iint_R dxdy}$$

High-Dimensional Integrals

Sample Integral from Statistical Physics

$$\langle U \rangle = \frac{1}{Z_N} \frac{1}{N!} \int dr^N U(r^N) e^{-\beta U(r^N)}$$

$3N_{particle}$ dimensional integral

- N=100 modest (course project)
  Therefore, in 3D, 300 dimensional integral
- Say 10 grid points in each dimension (very coarse)
  # function evaluations: 10^{300} (assume 1 flop)
- IBM BlueGene/L-system: 300 Tflop
- Total time: $10^{300}/10^{15} \sim 10^{285}$ s = 10^{277} years
- Age of the universe: 10^{14}
  # atoms on earth: 10^{50}

High-Dimensional Integrals

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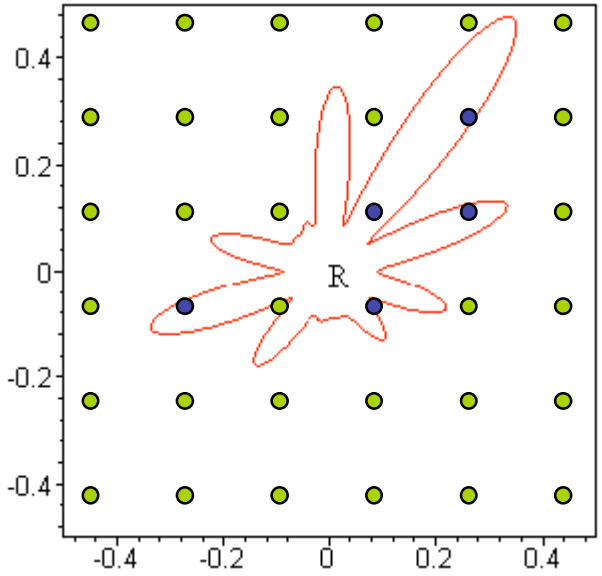
But we routinely compute such properties using MC

Integrate Over a Simple Shape? 1.

- Modify integrand to cast integral into a simple shaped region
  - *define a function indicating if inside or outside R*

$$\left\langle r^2 \right\rangle = \frac{\int_{-0.5}^{+0.5} dx \int_{-0.5}^{+0.5} dy (x^2 + y^2) s(x,y)}{\int_{-0.5}^{+0.5} dx \int_{-0.5}^{+0.5} dy s(x,y)}$$

$$s = \begin{cases} 1 & \text{inside R} \\ 0 & \text{outside R} \end{cases}$$

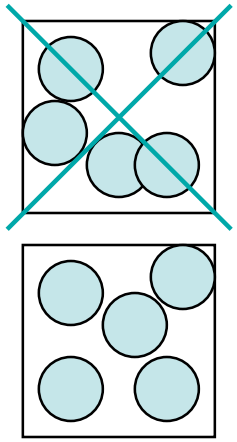


- Difficult problems remain
  - *grid must be fine enough to resolve shape*
  - *many points lie outside region of interest*
  - *too many quadrature points for our high-dimensional integrals (see applet again)*

•http://www.eng.buffalo.edu/~kofke/ce530/Applets/applets.html

Integrate Over a Simple Shape? 2.

- Statistical-mechanics integrals typically have significant contributions from miniscule regions of the integration space
  - $\langle U \rangle = \frac{1}{Z_N} \frac{1}{N!} \int dr^N U(r^N) e^{-\beta U(r^N)}$
  - *contributions come only when no spheres overlap*
  - *e.g., 100 spheres at freezing the fraction is 10^{-260}*



$\left(e^{-\beta U} \neq 0\right)$

- Evaluation of integral is possible only if restricted to region important to integral
  - *must contend with complex shape of region*
  - *MC methods highly suited to "importance sampling"*

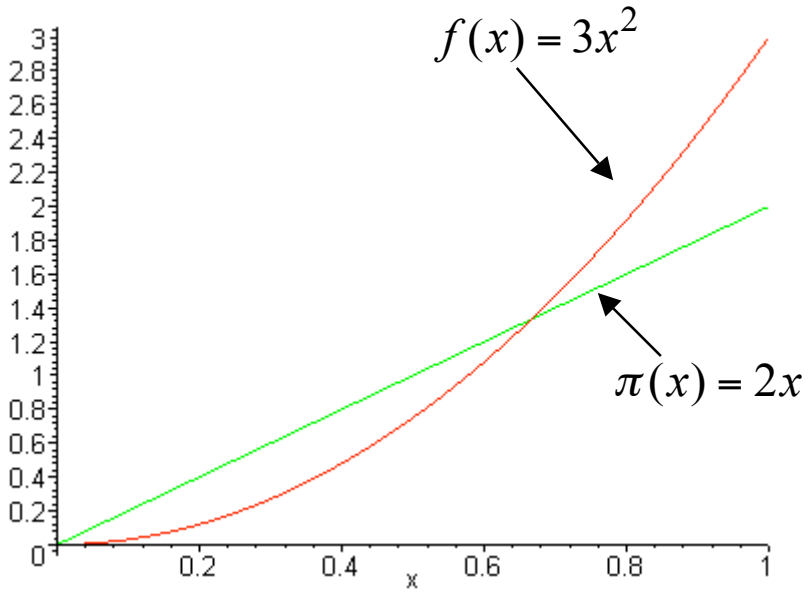
Importance Sampling

- Put more quadrature points in regions where integral receives its greatest contributions
- Return to 1-dimensional example

  Most contribution from region near x = 1

$$I = \int_0^1 3x^2 dx$$

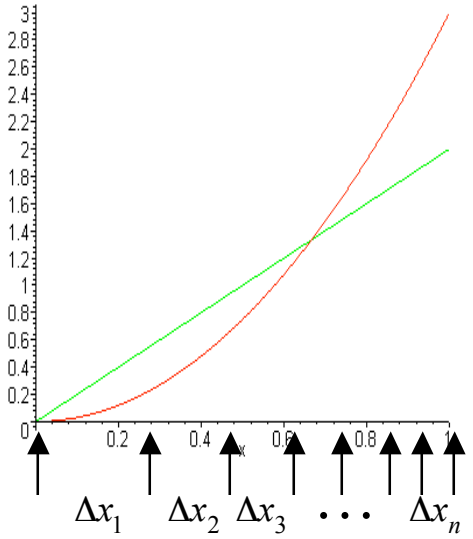
- Choose quadrature points not uniformly, but according to distribution $\pi(x)$
  - *linear form is one possibility*
- How to revise the integral to remove the bias?



The Importance-Sampled Integral

- Consider a rectangle-rule quadrature with unevenly spaced abscissas

$$I \approx \sum_{i=1}^{n} f(x_i)\Delta x_i$$



- Spacing between points
  - *reciprocal of local number of points per unit length*

$$\Delta x_i = \frac{b-a}{n}\frac{1}{\pi(x_i)}$$

Greater π(x) → more points → smaller spacing

- Importance-sampled rectangle rule
  - *Same formula for MC sampling*

$$I \approx \frac{b-a}{n}\sum_{\substack{i=1 \\ \pi(x)}}^{n} \frac{f(x_i)}{\pi(x_i)}$$

choose x points according to π(x)

The Importance-Sampled Integral

Error in MC is related to the variance:

$$\varepsilon^2 \approx \frac{\left\langle f^2 \right\rangle - \left\langle f \right\rangle^2}{n}$$

Can't control the $n^{-1/2}$ dependence

If f=constant, then numerator, and error vanish

Choose π to make f/π approximately constant, then can make error go to zero even if f is not constant.

$$\varepsilon^2 \approx \frac{\left\langle \left(\frac{f}{\pi} \right)^2 \right\rangle - \left\langle \left(\frac{f}{\pi} \right) \right\rangle^2}{n}$$

Generating Nonuniform Random Deviates

- Probability theory says...
  - ...given a probability distribution *u(z)*
  - if *x* is a function *x(z)*,
  - then the distribution of $\pi(x)$ obeys $\pi(x) = u(z)\left|\frac{dz}{dx}\right|$
- Prescription for $\pi(x)$
  - solve this equation for *x(z)*
  - generate *z* from the uniform random generator
  - compute *x(z)*
- Example
  - we want $\pi(x) = ax$ on *x* = (0,1)
  - then $z = \frac{1}{2}ax^2 + c = x^2$ *a and c from "boundary conditions"*
  - so $x = z^{1/2}$
  - taking square root of uniform deviate gives linearly distributed values
- Generating $\pi(x)$ requires knowledge of $\int \pi(x)dx$

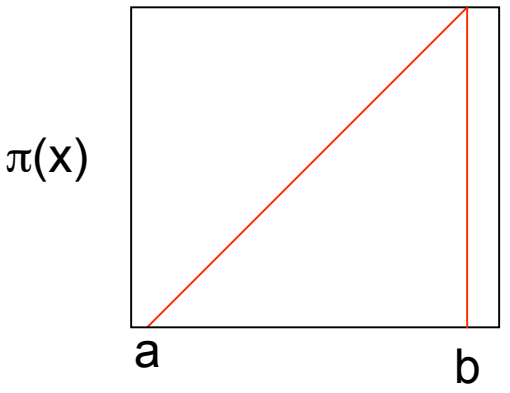
Generating Nonuniform Random Deviates

Example:

Generate x from linearly distributed random numbers between [a,b), $\pi(x)$

If $\pi(x)$ is normalized then,

$$\pi(x) = \frac{2x}{b^2 - a^2}$$

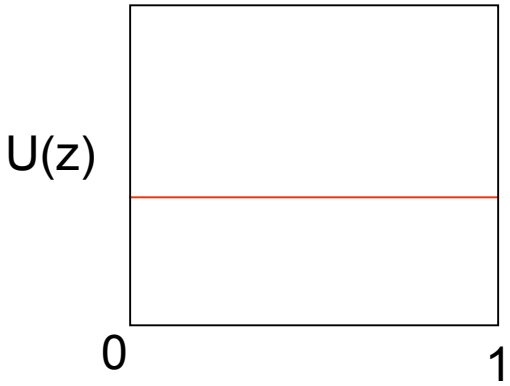


If we have u(z) a uniform random number [0,1)

$$\pi(x) = \frac{2x}{b^2 - a^2} = 1\frac{dz}{dx}$$

$$\int_a^x dx \frac{2x}{b^2 - a^2} = \int_0^z dz$$

$$x = \sqrt{a^2 + (b^2 - a^2)z}$$

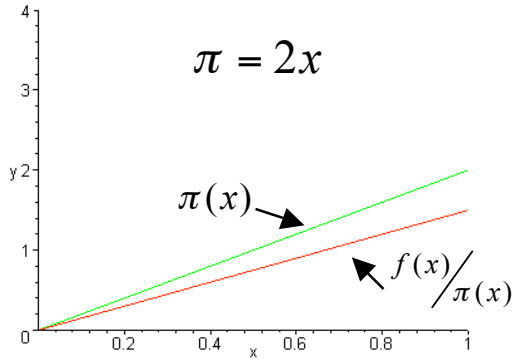


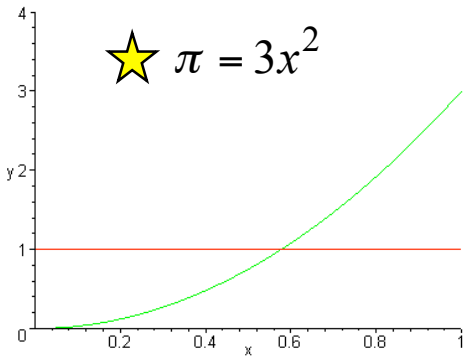
Choosing a Good Weighting Function

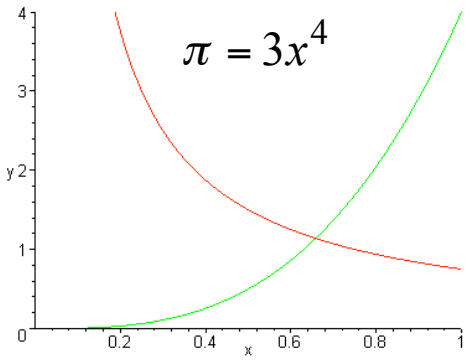
- MC importance-sampling quadrature formula

$$I \approx \frac{1}{n} \sum_{i=1}^{n} \frac{f(x_i)}{\pi(x_i)}$$
$$\pi(x)$$

- Do not want $\pi(x)$ to be too much smaller or too much larger than f(x)
  - too small leads to significant contribution from poorly sampled region
  - too large means that too much sampling is done in region that is not (now) contributing much







Variance in Importance Sampling Integration

- Choose π to minimize variance in average

$$\sigma_I^2 = \frac{1}{n}\left\{\int\left[\frac{f(x)}{\pi(x)}\right]^2 \pi(x)dx - \left[\int\left[\frac{f(x)}{\pi(x)}\right]\pi(x)dx\right]^2\right\}$$

$f(x) = 3x^2$

$\pi(x)$	σ_I	n = 100	n = 1000
1	$2/\sqrt{5n}$	0.09	0.03
$2x$	$1/\sqrt{8n}$	0.04	0.01
$3x^2$	0	0	0
$4x^3$	$1/\sqrt{8n}$	0.04	0.01

- Smallest variance in average corresponds to $\pi(x) = c \times f(x)$
  - *not a viable choice*
  - *the constant here is selected to normalize $\pi(x)$*
  - *if we can normalize $\pi(x)$ we can evaluate $\int \pi(x)dx$*
  - *this is equivalent to solving the desired integral of f(x)*

- http://www.eng.buffalo.edu/~kofke/ce530/Applets/applets.html

Summary

- Monte Carlo methods use stochastic process to answer a non-stochastic question
  - generate a random sample from an ensemble
  - compute properties as ensemble average
  - permits more flexibility to design sampling algorithm
- Monte Carlo integration
  - good for high-dimensional integrals
    - better error properties
    - better suited for integrating in complex shape
- Importance Sampling
  - focuses selection of points to region contributing most to integral
  - selecting of weighting function is important
  - choosing perfect weight function is same as solving integral

Extra Slides

Approximate function with Polynomial

Recall, that the interpolating polynomial depends on the chosen grid points

$$P_n(x) = \sum_{i=0}^{n} l_i(x) f(x_i)$$

Langrange interpolants can be written as,

$$l_i(x) = \frac{\alpha(x)}{(x - x_i)\alpha'(x_i)}$$

$$\alpha(x) = (x - x_1)(x - x_2)..(x - x_n) = \prod_{i=0}^{n} (x - x_i)$$

$$\alpha'(x_i) = \prod_{\substack{j=0 \\ j \neq i}}^{n} (x_i - x_j)$$

Note that here, $\lim_{x \to x_i} l_i(x) = \lim_{x \to x_i} \frac{\alpha(x)}{(x - x_i)\alpha'(x_i)} = 1$

Theorem (Gauss)

Let *P(x)* be a nontrivial polynomial of degree *n* such that it is orthogonal to polynomials of lesser degree

$$\int_a^b x^k P(x)dx = 0 \qquad 0 \le k \le n-1$$

If $x_0, x_1, x_2, \ldots x_n$ are zeros of *P(x)* and

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

Then this approximation is exact for all polynomials of degree less than or equal to *2n+1*

Method 2:

In practice, we use Gauss' Theorem and well-studied classes of orthogonal polynomials

Here, Legendre Polynomials (hence sometimes Gauss-Legendre Quadrature)

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \frac{2}{2n+1}\delta_{nm}$$

All we do are look for zeros of $P_n(x)$ in *[-1,1].* These are our x_is.

The c_is can be obtained from

$$c_i = \frac{2}{(1-x_i^2)(P_n'(x_i))^2}$$