Comments on singularities
Open-interval formulas can be used
- singular point(s) should be at end(s); divide up interval in parts if needed
- but convergence with number of points n may be very slow
Divergent part can some times be subtracted and solved analytically
More sophisticated methods exist for difficult cases

Other methods
Gaussian quadrature:
- non-uniform grid points; n+1 points → exact result for polynomial of order n
- several Julia packages, e.g., FastGaussQuadrature.jl

Gauss-Kronrod quadrature:
- uses two Gaussian quad. evaluations for different n, similarly to Romberg
- package QuadGK.jl uses a version of this method

Adaptive grid (adaptive mesh):
- dynamically adapted to be more dense where most needed

Infinite integration range
Change variables to make range finite
**Multi-Dimensional integration**

\[
I = \int_{a_n}^{b_n} dx_n \cdots \int_{a_2}^{b_2} dx_2 \int_{a_n}^{b_n} dx_1 f(x_1, x_2, \ldots, x_n),
\]

Can be carried out numerically dimension-by-dimension

Example, function of two variables

\[
I = \int_{a_y}^{b_y} dy \int_{a_x(y)}^{b_x(y)} dx f(x, y)
\]

Integrating numerically over \(x\) first, gives a function of \(y\):

\[
F(y) = \int_{a_x(y)}^{b_x(y)} dx f(x, y)
\]

This has to be done for values of \(y\) on a grid, to be used in

\[
I = \int_{a_y}^{b_y} dy F(y)
\]

Very time consuming for large dimensionality \(D\); scaling \(M^D\) of effort

- \(M\) represents mean (geom) number of grid points for 1D integrals
Monte Carlo Integration

An integral over a finite volume $V$:
- is (by definition) the mean value of the function times the volume

$$I = \int_{a}^{b} f(x)dx = (b - a)\langle f \rangle$$

The mean value $\langle f \rangle$ can be estimated by sampling
- generate $N$ random (uniformly distributed) $x$ values $x_i$ in the range, then

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \to \langle f \rangle, \text{ when } N \to \infty$$

For finite $N$, there is a statistical error:

$$\langle \bar{f} - \langle f \rangle \rangle \propto \frac{1}{\sqrt{N}}$$

The statistical result for the integral should be expressed as

$$I = \bar{I} \pm \sigma = V(\bar{f} + \sigma/V) \quad \sigma \propto N^{-1/2}$$

Computing the “error bar” $\sigma$ is an important aspect of the sampling method

Interpretation of the mean error:
If the “simulation” is repeated many times, the averaged squared error (variance) tends to a value $a/N$, for with $a$ some constant.
Consider a circle of radius 1, centered at \((x,y)=0\). Define a function:

\[
f(x, y) = \begin{cases} 
1, & \text{if } x^2 + y^2 \leq 1 \\
0, & \text{if } x^2 + y^2 < 1
\end{cases}
\]

Use MC sampling to compute:

\[A = \int_{-1}^{1} dy \int_{-1}^{1} dx f(x, y) = \pi = 4 \langle f \rangle\]

Expected fraction of “hits” inside circle = \(\pi/4\)

We should compute the statistical error properly
**Statistical errors**

Expressing a statistical estimate as \( A \pm \sigma \), the meaning normally is:
- \( \sigma \) represents one standard deviation of the computed mean value \( A \)
- under the assumption of normal-distributed fluctuations

Then, the probability of the true value being
- within \([A-\sigma,A+\sigma]\) is 68%
- within \([A-2\sigma,A+2\sigma]\) is 95%
- within \([A-3\sigma,A+3\sigma]\) is 99.7%

For \( M \) independent samples \( A_i \):

\[
\bar{A} = \frac{1}{M} \sum_{i=1}^{M} A_i
\]

\[
\sigma_A = \sqrt{\frac{1}{M} \sum_{i=1}^{M} (A_i - \bar{A})^2} = \sqrt{\frac{1}{M} \sum_{i=1}^{M} A_i^2 - \bar{A}^2} = \sqrt{\bar{A}^2 - (\bar{A})^2}
\]

This is the standard deviation of the distribution of values \( \{A_i\} \)

But the “error bar” is the standard deviation of the mean of \( \{A_i\} \)
The mean value fluctuates less than the width \( \sigma_A \) of the distribution
- imagine taking the number of samples \( M \) to infinity:

\[
\sigma_A = \sqrt{\frac{1}{M} \sum_{i=1}^{M} (A_i - \bar{A})^2}
\]
will approach a constant value
- the standard deviation of the distribution

\[
\bar{A} = \frac{1}{M} \sum_{i=1}^{M} A_i
\]
will approach a constant value
- the actual value \( \langle A \rangle \) of \( A \)

Variances add: variance of the sum \( \sum_{i=1}^{M} A_i \) is \( M \sigma_A^2 \)
- standard deviation of the sum is \( \sqrt{M} \sigma_A \)
- divide by \( M \); standard deviation of the mean is \( \sigma_A / \sqrt{M} \)
- here \( M \) should be replaced by \( M-1 \) (reflecting infinite uncertainty if \( M=1 \))

\[
\sigma = \sqrt{\frac{1}{M(M-1)} \sum_{i=1}^{M} (A_i - \bar{A})^2} = \sqrt{\frac{1}{M(M-1)} \sum_{i=1}^{M} (A_i^2 - \bar{A}^2)} = \sqrt{\frac{A^2 - (\bar{A})^2}{M - 1}}
\]
**Data binning**

The statistical error ("error bar") has its conventional meaning only if the values \{A_i\} are normal distributed
- typically they obey some completely different distribution

Apply central limit theorem to obtain normal distributed "bin averages"

A bin average is based on M samples as before, but now B of them
- B different mean values (estimates of A): \(\bar{A}_1, \bar{A}_2, \ldots, \bar{A}_B\)

\[
\bar{A}_b = \frac{1}{M} \sum_{i=1}^{M} A_{b,i} \quad \text{A}_{b,i} \text{ is value } i \text{ belonging to bin } b
\]

Regardless of the distribution of individual values
- if M is large enough, the bin averages are normal-distributed

Use standard formulas with the bin data:

\[
\bar{A} = \frac{1}{B} \sum_{b=1}^{B} \bar{A}_b \quad \sigma = \sqrt{\frac{1}{B(B-1)} \sum_{b=1}^{B} (\bar{A}_b - \bar{A})^2} = \sqrt{\frac{1}{B(B-1)} \sum_{b=1}^{B} (\bar{A}_b^2 - \bar{A}^2)} = \sqrt{\frac{A^2 - (\bar{A})^2}{B - 1}}
\]
Emergence of normal distribution
- example: sampling f=1 circle in square
- let's just consider the estimate of the mean \( \langle f \rangle \)

For each sample, the probabilities of \( f=0,1 \) are:

\[
P(f = 1) = \pi/4, \quad P(f = 0) = 1 - \pi/4
\]

For \( N \) samples, the possible average values \( A \) are

\[
A \in \left\{0, \frac{1}{N}, \frac{2}{N}, \ldots, \frac{N-1}{N}, 1\right\}
\]

the probabilities of these averages are

\[
P\left(A = \frac{m}{N}\right) = \frac{N!}{m!(N-m)!} \left(\frac{\pi}{4}\right)^m \left(1 - \frac{\pi}{4}\right)^{N-m}
\]
Evolution of $P(A)$ from $N=1$ to 100

Note: We can think of the probability distribution of a continuum of $A$ values

Sum of delta-functions reflects discrete set of possible values

For large $N$, a small broadening of the deltas (e.g., bars or Gaussians) give a continuous distribution

$$P(A) = \sum_{m=0}^{N} \frac{N!}{m!(N-m)!} \left(\frac{\pi}{4}\right)^m \left(1 - \frac{\pi}{4}\right)^{N-m} \delta(A - m/N)$$