Numerical integration on a mesh vs MC sampling

Scaling of the computational effort:

- may depend on the dimensionality and the required precision ε

Mesh-based method: time ~ $M(\varepsilon)^D \times g(\varepsilon)$

- where $g(\varepsilon)$ depends on integrand and method

Monte Carlo sampling method: $\varepsilon \sim N^{-1/2}$, time ~ $\varepsilon^{-2} \times h(f)$

- where h(f) depends on the function f
- time scaling not explicitly dependent on the dimensionality D

Which type of method is better?

- for given desired precision ε

The above scaling forms show that MC sampling should be better above some dimensionality D

- in practice, mesh-based methods are difficult even for D=3
- MC sampling can work well even in very high dimensions
  - unless the integrand is strongly varying (low probability of hitting contributing parts of the volume

Example: modified circle integration

Function with singularity. Inside circle of radius 1:

$$f(r) = r^{-\alpha}, \quad r = \sqrt{x^2 + y^2}$$

integrable if $\alpha < 2$

$$I = \int_{-1}^{1} dy \int_{-1}^{1} dx f(x, y), \quad f(x, y) = r^{-\alpha}, \text{ if } r \leq 1, \quad f(x, y) = 0, \text{ if } r > 1$$

Distribution of radius r inside circle: ***P(r)=2r*** ***(0 ≤ r ≤ 1)***

$$\int_0^1 P(r)dr = 2\int_0^1 rdr = 1$$

Distribution of function values inside the circle:

$$P(f)df = P(r)\left|\frac{dr}{df}\right| df = \frac{2}{\alpha} f^{-1-2/\alpha} df$$

outside:

$$P(f) = (1 - \pi/4)\delta(f)$$

$$P(f) = \frac{\pi}{4}\frac{2}{\alpha} f^{-1-2/\alpha}\Theta(f-1) + \left(\frac{\pi}{4} - 1\right)\delta(f)$$

Distribution of average A of f based on N samples:

$$P(A) = \int_0^\infty df_N \cdots \int_0^\infty df_1 P(f_N) \cdots P(f_1)\delta[A - (f_1 + \cdots + f_N)/N]$$

$$P(A) = \int_0^\infty df_N \cdots \int_0^\infty df_1 P(f_N) \cdots P(f_1) \delta[A - (f_1 + \cdots + f_N)/N]$$

Should become normal distribution for large N

What is large enough (e.g., to use for data binning)?

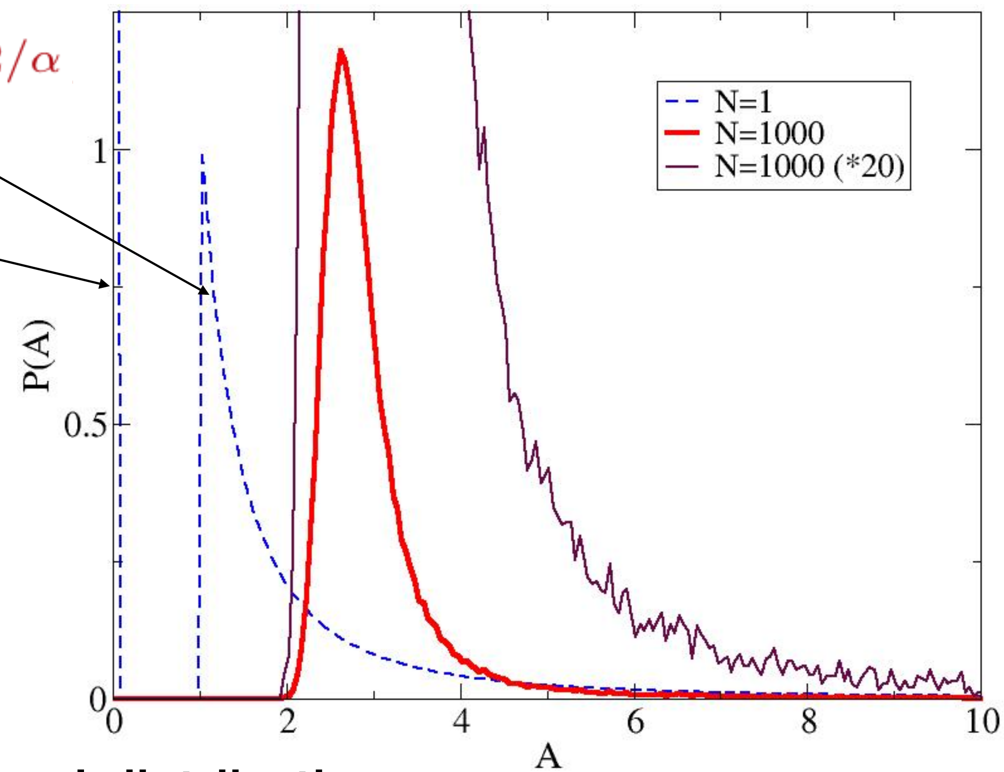
How can we compute the probability distribution?

Monte Carlo sampling
- we can get P(A)
- not just <A>

$$\frac{2}{\alpha} f^{-1-2/\alpha}$$

$$\delta(f)$$

$$\alpha = 3/2$$



There is a delta fktn at A=0 in the N=1000 result, with a very small amplitude $(1-\pi/4)^{1000}$

For N=1000, there is still a “fat tail”

- larger N needed to approximte normal distribution

What happens if the function is not integrable?

Example: boarderline case: $f(r) = r^{-\alpha}, \alpha = 2$

- singularity at r=0, log divergence vs lower cut-off r_0

$$\int_0^{2\pi} d\phi \int_{r_0}^{1} \frac{r\,dr}{r^2} = -2\pi \ln(r_0) = 2\pi \ln(1/r_0)$$

How is the divergence manifested in MC sampling?

Rare-event behavior
- due to fat tails in P(A)

Occasional very large f values give huge contributions to A, cause spikes in A(N)

The overall behavior of <A(N)>, i.e., the peak of the of distribution of P(A(N)), shows a log behavior

Four independent simulations
- partial averages based on N samples