Monte Carlo Integration 2

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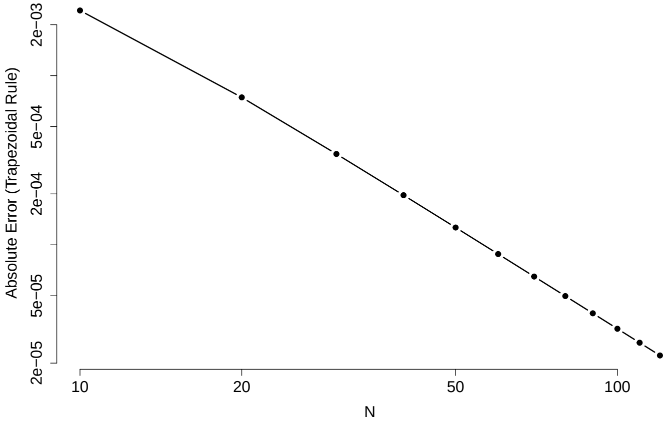
Why use Monte Carlo integration at all?

Apply Trapezoidal Rule to $I = \frac{1}{\sqrt{2\pi}} \int_3^\infty e^{-x^2/2} dx$:



- Trapezoidal Rule: Absolute error of $\sim 1 \times 10^{-5}$ with only about 100 points.
- Gaussian Quadrature: far better approximation in far fewer # of points!

Then why use Monte Carlo integration at all?

Error behaviour: Numerical integration in 1 dimension

Consider approximating integral of a function f of a *single* variable x:

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

Error in the numerical approximation:

$$\epsilon \propto \delta^k,$$

where the grid spacing

$$\delta = (b - a)/n$$

and k (*order* of the integration method) is 2 for trapezoidal, 3 or 4 for Simpson, etc.

Because

$$\delta \propto n^{-1},$$

we have

$$\epsilon \propto n^{-k}.$$

Error behaviour: Numerical integration in d dimensions

Consider approximating integral of a function f of d variables $x_1, \ldots, x_d$:

$$I = \int \ldots \int g(x_1, \ldots, x_d) dx_1, \ldots, dx_d$$

Error in the numerical approximation (trapezoidal, Simpson, etc.)

$$\epsilon \propto \delta^k.$$

Now, the grid size along any dimension is

$$\delta^d \propto n^{-1}, \text{ that is, } \delta \propto n^{-1/d}.$$

Hence

$$\epsilon \propto n^{-k/d}.$$

Larger the d, slower the convergence! Curse of Dimensionality

Multi-dimensional integral

$$\begin{aligned} I &= \int \dots \int g(x_1, \dots, x_d) dx_1, \dots, dx_d \\ &= \int \dots \int h(x_1, \dots, x_d) f(x_1, \dots, x_d) dx_1, \dots, dx_d \end{aligned}$$

with

$$\begin{aligned} f(x_1, \dots, x_d) &\geq 0 \\ \int \dots \int f(x_1, \dots, x_d) dx_1, \dots, dx_d &= 1 \\ h(x_1, \dots, x_d) f(x_1, \dots, x_d) &= g(x_1, \dots, x_d) \end{aligned}$$

for each $(x_1, \dots, x_d)$.

Algorithm

1. Generate $(X_1^{(1)}, X_2^{(1)}, \ldots, X_d^{(1)}), \ldots, (X_1^{(n)}, X_2^{(n)}, \ldots, X_d^{(n)}) \sim f$
2. Estimator I as $\widehat{I}_n = \frac{1}{n}\sum_{i=1}^{n} h(X_1^{(i)}, \ldots, X_d^{(i)})$
3. $\widehat{\text{Var}}\left(\widehat{I}_n\right) = \frac{1}{n} \times \frac{1}{n-1}\sum_{i=1}^{n}\left(h(X_1^{(i)}, \ldots, X_d^{(i)}) - \widehat{I}_n\right)^2$
4. Etc.

Error behaviour: Monte Carlo integration in d dimensions

Because we *estimate* the value of I
the error in the estimate is expected to be

$$O(n^{-1/2})$$

independent of the # of dimensions!

Error behaviour: Monte Carlo integration in d dimensions

For any k (i.e., order of the numerical integration method), for sufficiently large number d of dimensions, we will have

$$k/d < 1/2.$$

This means that, beyond this value of d; i.e., for

$$d > 2k,$$

the error in numerical approximation will be more than that in the Monte Carlo estimate.

more pointers here

Monte Carlo integration is therefore particularly useful when dealing with high-dimensional integrals. High-dimensional integrals often occur in statistical physics, Bayesian inference, etc.

Toy example

Estimating / approximating
volume of d-dimensional unit hypersphere

Statutory Warning

High-dimensional spaces and objects

can be

strange

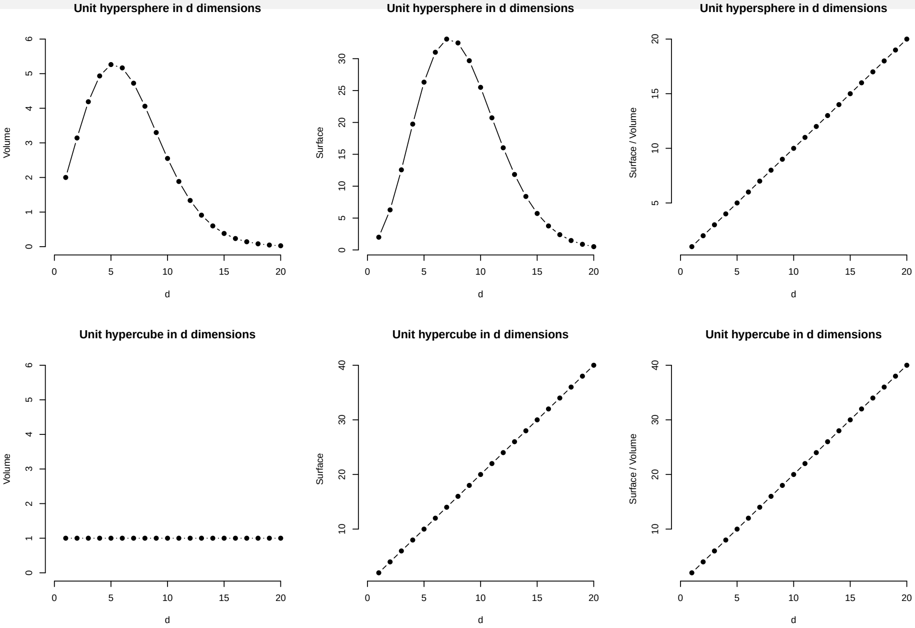
and

injurious to intuition from 3 dimensions

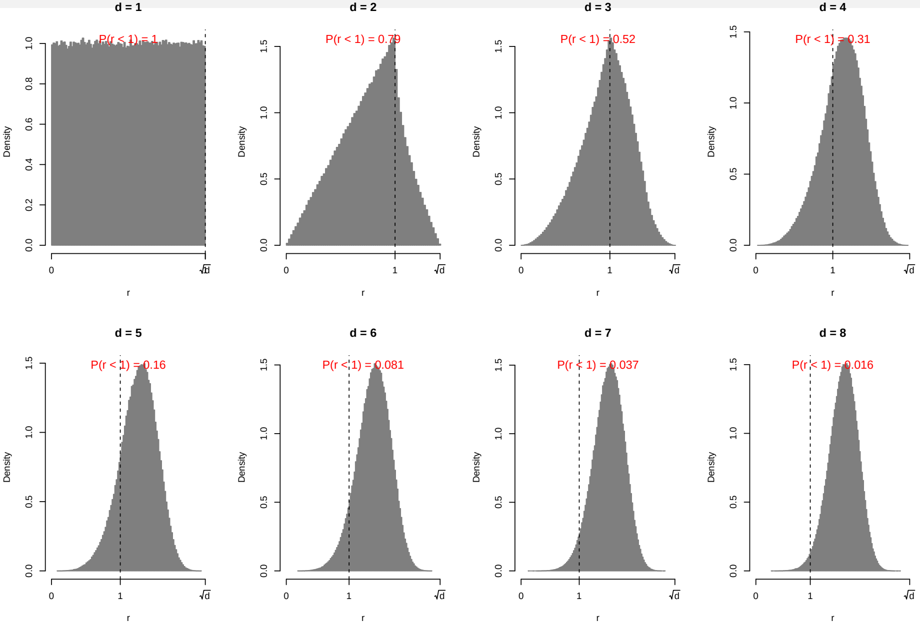
Hypershperes and hypercubes in d dimensions

	Volume	Surface
Hypercube	L^d	$2dL^{d-1}$
Hypersphere	$\frac{\pi^{\frac{d}{2}}}{\Gamma\left(1+\frac{d}{2}\right)}R^d$	$\frac{\pi^{\frac{d}{2}}}{\Gamma\left(1+\frac{d}{2}\right)}dR^{d-1}$

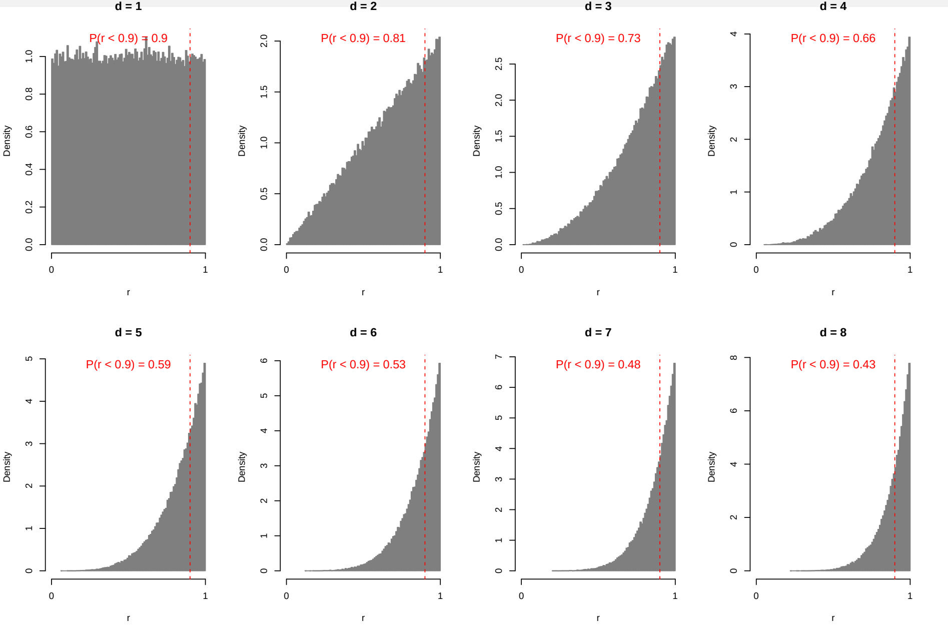
Hypershperes and hypercubes in d dimensions



Distance distribution inside unit d-hypercubes



Distance distribution inside unit d-hyperspheres



20-dimensional watermelons

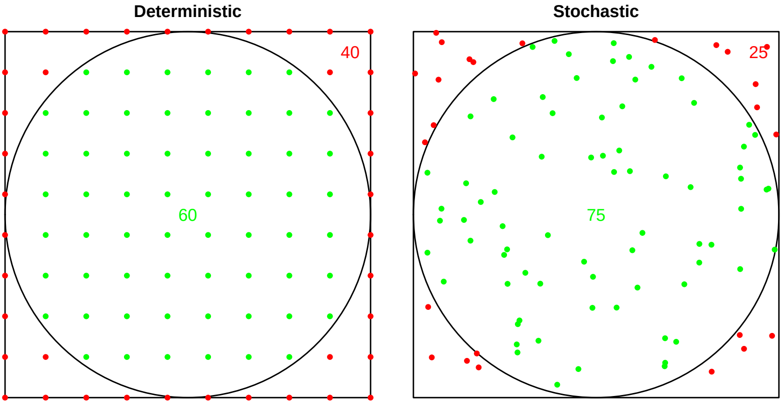
5.14. A property of the n-dimensional volume. It consists in the fact that for very large n the "*volume of an n-dimensional figure is concentrated near its surface.*" For example, the volume of the spherical ring between spheres of radius 1 and $1-\epsilon$ equals $b_n[1-(1-\epsilon)^n]$, which, for fixed arbitrarily small ϵ, but increasing n approaches b_n. A 20-dimensional watermelon with a radius of 20 cm. and a skin with a thickness of 1 cm. is nearly two-thirds skin:

$$1-\left((1-\frac{1}{20}\right)^{20}\approx 1-e^{-1}.$$

p.124
Kostrikin & Manin
Linear Algebra & Geometry
Gordon & Breach Science Publishers (1989?)

Courtesy: Prof. Anil Gangal

Estimating volume: deterministic & stochastic dartboards



$$\text{Area approximation or estimate} = 4 \times \frac{\#\text{ of points inside }\bigcirc}{\#\text{ of points inside }\square}.$$

Volume of d-dimensional unit hypersphere: MCI

Formally,

$$
\begin{aligned}
V(d) &= 2^d \int_0^1 \dots \int_0^1 h(x_1, \dots, x_d) dx_1 \dots dx_d \\
&= 2^d \int \dots \int h(x_1, \dots, x_d) f(x_1, \dots, x_d) dx_1 \dots dx_d,
\end{aligned}
$$

where

$$
\begin{aligned}
h(x_1, \dots, x_d) &= \begin{cases} 1 & \sum_{i=1}^d x_i^2 \le 1 \\ 0 & \text{otherwise} \end{cases} \\
f(x_1, \dots, x_d) &= \begin{cases} 1 & 0 \le x_1, \dots, x_d \le 1 \\ 0 & \text{otherwise} \end{cases}.
\end{aligned}
$$

$f(x_1, \dots, x_d)$ :: uniform PDF over d-dimensional unit hypercube

Algorithm

1. Generate $(X_1^{(1)}, X_2^{(1)}, \ldots, X_d^{(1)}), \ldots, (X_1^{(n)}, X_2^{(n)}, \ldots, X_d^{(n)}) \sim f$
2. Estimator $V(d)$ as $\widehat{V}_n(d) = \frac{1}{n} \sum_{i=1}^{n} h(X_1^{(i)}, \ldots, X_d^{(i)})$
3. $\widehat{\text{Var}}\left(\widehat{V}_n(d)\right) = \frac{1}{n} \times \frac{1}{n-1} \sum_{i=1}^{n} \left(h(X_1^{(i)}, \ldots, X_d^{(i)}) - \widehat{V}_n(d)\right)^2$
4. Etc.

Effectively, step 2 yields

$$\widehat{V}_n(d) = 2^d \times \frac{\#\text{ of points inside } \bigcirc}{\#\text{ of points inside } \square}.$$

To do ...

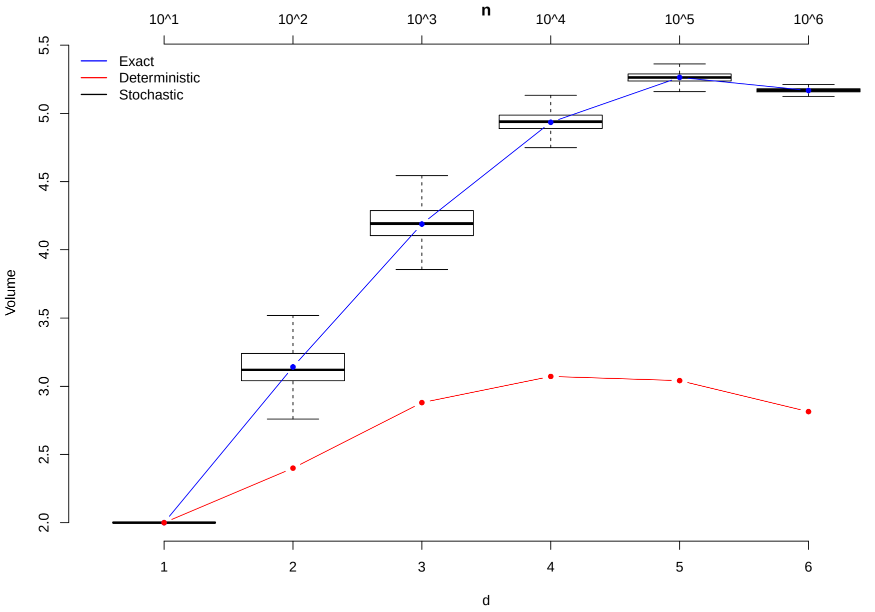
Let us now

- apply this MCI estimator to the deterministic and stochastic grids;
- compare results the exact volume volume of a d-dimensional unit hypersphere:

$$V(d) = \frac{\pi^{\frac{d}{2}}}{\Gamma\left(1 + \frac{d}{2}\right)};$$

- compare stochastic and deterministic results for the same n and d.

Deterministic vs. stochastic dartboard comparison



Hypersphere volume estimation using MCI: A surprise

$\widehat{\mathrm{SE}}\left(\widehat{V}_n(d)\right) \approx d^2$ :: not constant :: not clear why