Introduction to Monte Carlo

An integration example

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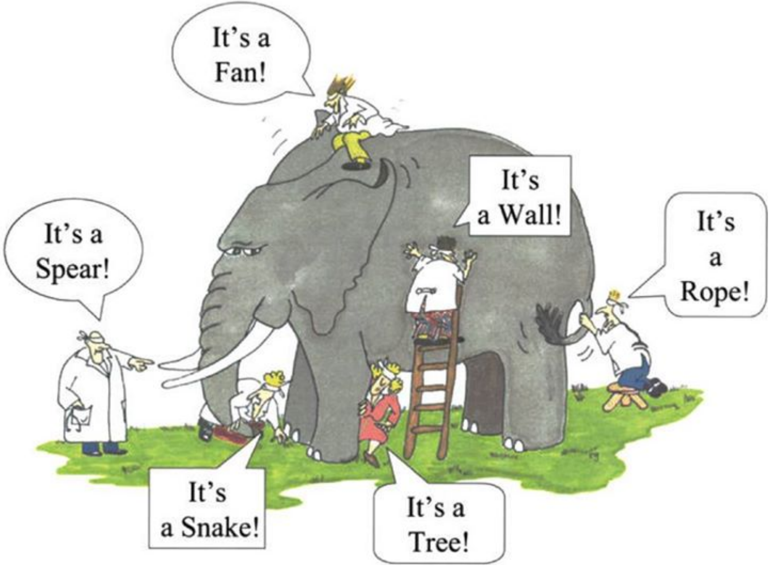

Monte Carlo is different things to different people

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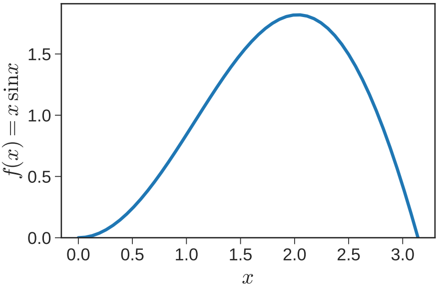
Example

Consider the particular 1D integral

$$I = \int_0^{\pi} x \sin x \; dx.$$



$$I = \int_0^{\pi} x \sin x \; dx = -x\cos(x) + \sin(x)\big|_0^{\pi} = \pi.$$

Average Value and Integral

The average value $\bar{f}$ is the mean "height" of the function.

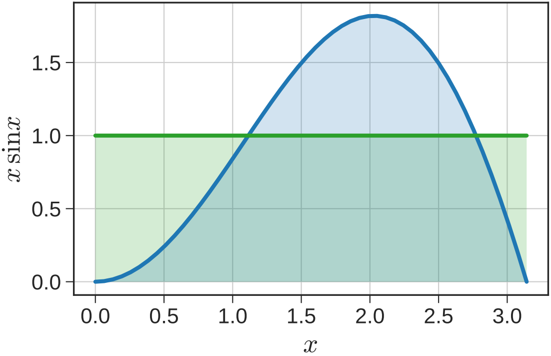
$$\begin{aligned} \bar{f} &= \frac{\int_a^b f(x)dx}{\int_a^b dx} \\ &= \frac{\int_a^b f(x)dx}{b-a} \\ &= \frac{I}{b-a} \end{aligned}$$

Therefore, integral $=$ average $\times$ domain size

$$I = \bar{f}(b-a)$$

In our example, $\bar{f} = 1$. Hence, $I = 1(\pi - 0) = \pi$.

The areas under the blue and green curves are equal.



Insight: integral $\leftrightarrow$ average value of the integrand

Average Value

Method 1:

- pick n uniformly spaced points x_i in the domain
- evaluate the average:

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

Method 2:

- select n randomly chosen points x_i in the domain
- evaluate the average:

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

Computing Average Value

```
def equispacedAverage(npts):
    xi = np.linspace(0, np.pi, npts)
    fi = xi * np.sin(xi)
    return np.mean(fi)

def randomAverage(npts):
    xi = np.random.uniform(0, np.pi, npts)
    fi = xi * np.sin(xi)
    return np.mean(fi)
```

Let us test the two subroutines.

Recall that the true $\bar{f} = 1$.

Computing Average Value

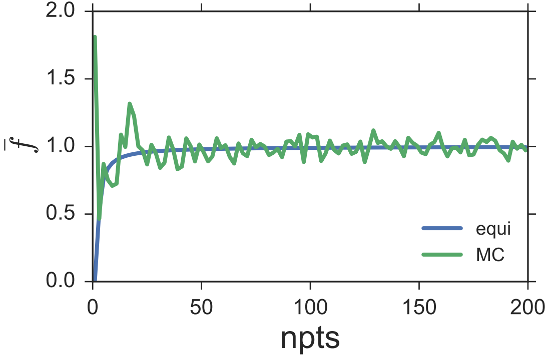
```
npts = 10; print(equispacedAverage(npts))
0.890842865047
```

```
npts = 10; print(randomAverage(npts))
0.812445848056
```

Reasonable enough.

Let us now systematically vary `npts` between 1 and 200.

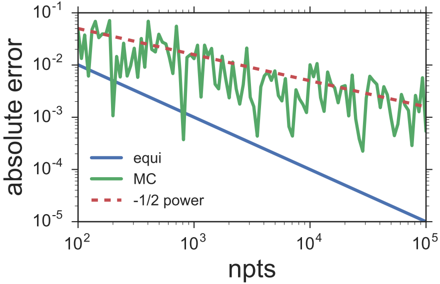
Equispaced versus Random



- As `npts` $\uparrow$, both estimates "converge" to $\bar{f} = 1$ (why?)
- Method 1 converges more "systematically" (why?)
- Random requires more work (generate random numbers), and produces an inferior answer.

Convergence in 1D

Consider the absolute error $\epsilon = |\bar{f}_{\text{true}} - \bar{f}_{\text{est}}|$,



Convergence in general,

$$\epsilon_{\text{equi}} \sim \frac{1}{n}; \epsilon_{\text{mc}} \sim \frac{1}{\sqrt{n}}$$

Insight: For 1D integrals, MC is a bad idea!

2D Integrals: "integration by darts"

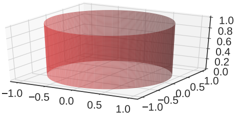
Classic problem: area of a circle

Mathematically,

$$I = \int_{-1}^{1} \int_{-1}^{1} g(x_1, x_2) dx_1 dx_2,$$

where,

$$g(x_1, x_2) = \begin{cases} 1, & \text{if } x_1^2 + x_2^2 \leq 1 \\ 0, & \text{otherwise.} \end{cases}$$



$$\text{integral} = \text{average} \times \text{domain size}$$

$$I = \bar{g} \times (2 \times 2) = 4\bar{g}$$

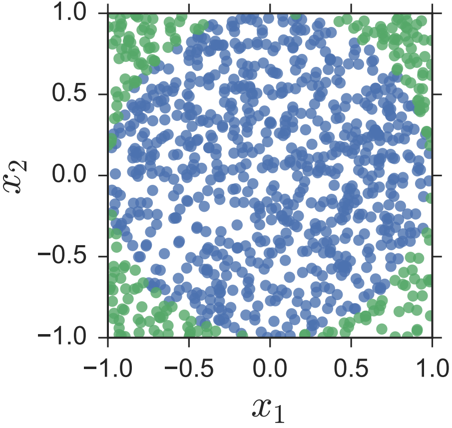
Note: True $I = \pi; \bar{g} = \pi/4$

Python

```python
def MCdarts(npts):

    """input : #darts,
       output: average value of g"""

    x1 = np.random.uniform(-1,1,size=npts)
    x2 = np.random.uniform(-1,1,size=npts)

    cond = x1**2 + x2**2 <= 1

    return np.sum(cond)/float(npts)
```

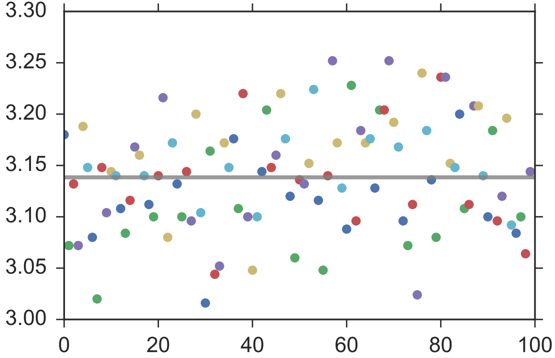
Let us throw 1000 darts:

```
print("area", 4*MCdarts(1000))
area 3.148
```



Variability

Repeat experiment of throwing 1000 darts many (=100) times:



Insight: need to account for variability when analyzing MC

Equispaced Analog

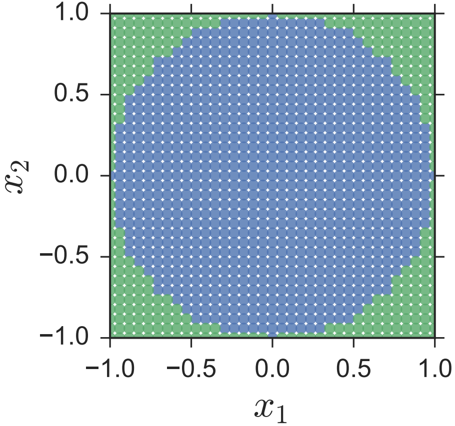
Now, let us throw darts systematically on a "grid"

```
def equiDarts(npts, isPlot=False):
    """total number of points are npts = ngrid*ngrid"""

    ngrid = int(np.sqrt(npts))

    x = np.linspace(-1, 1, ngrid)
    x1, x2 = np.meshgrid(x,x)

    cond = x1**2 + x2**2 <= 1

    y = np.sum(cond,axis=0)
    y = np.sum(y)

    return y/float(npts)
```

Darts on a Regular Grid

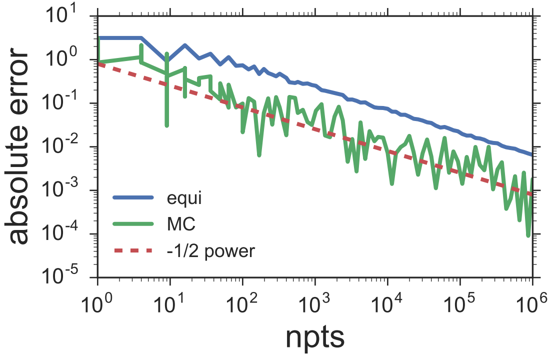
Use 1000 darts ($\sqrt{1000} \approx 35$).

```
print("area", 4*equiDarts(1000))
area 2.94204081633
```



This is worse than most of the MC answers.

Convergence



1. The error in both methods $\epsilon \sim n^{-1/2}$.
2. ϵ_{equi} no longer decays smoothly, especially initially
3. ϵ_{mc} is lower than ϵ_{equi}

Curse of Dimensionality

In fact, it can be shown that,

$$\epsilon_{\mathsf{mc}} \sim n^{-1/2}, \quad \text{independent of dimension.}$$

For *any* systematic "quadrature" method,[1]

$$\epsilon_{\mathsf{quad}} \sim n^{-p_{1D}/d},$$

where p_{1D} is the convergence of the method for 1D problems.

This is called the curse of dimensionality.

Many important computational problems are high-dimensional.

[1] not just equispaced; rectangle, trapezoidal, Simpson's have $p_{1D} = 1$, 2, and 4, respectively.

Summary

- integral = average $\times$ domain size;
- For 1D averages, MC is a bad idea;
- For higher dimensional integrals, standard quadrature methods suffer from the curse of dimensionality;
- For higher dimensional integrals, the error in MC decreases as the square root of the number of samples due to the central limit theorem;
- estimates from MC are noisy