Physics takes a gamble!
The science behind Monte Carlo methods

A chance-driven computation

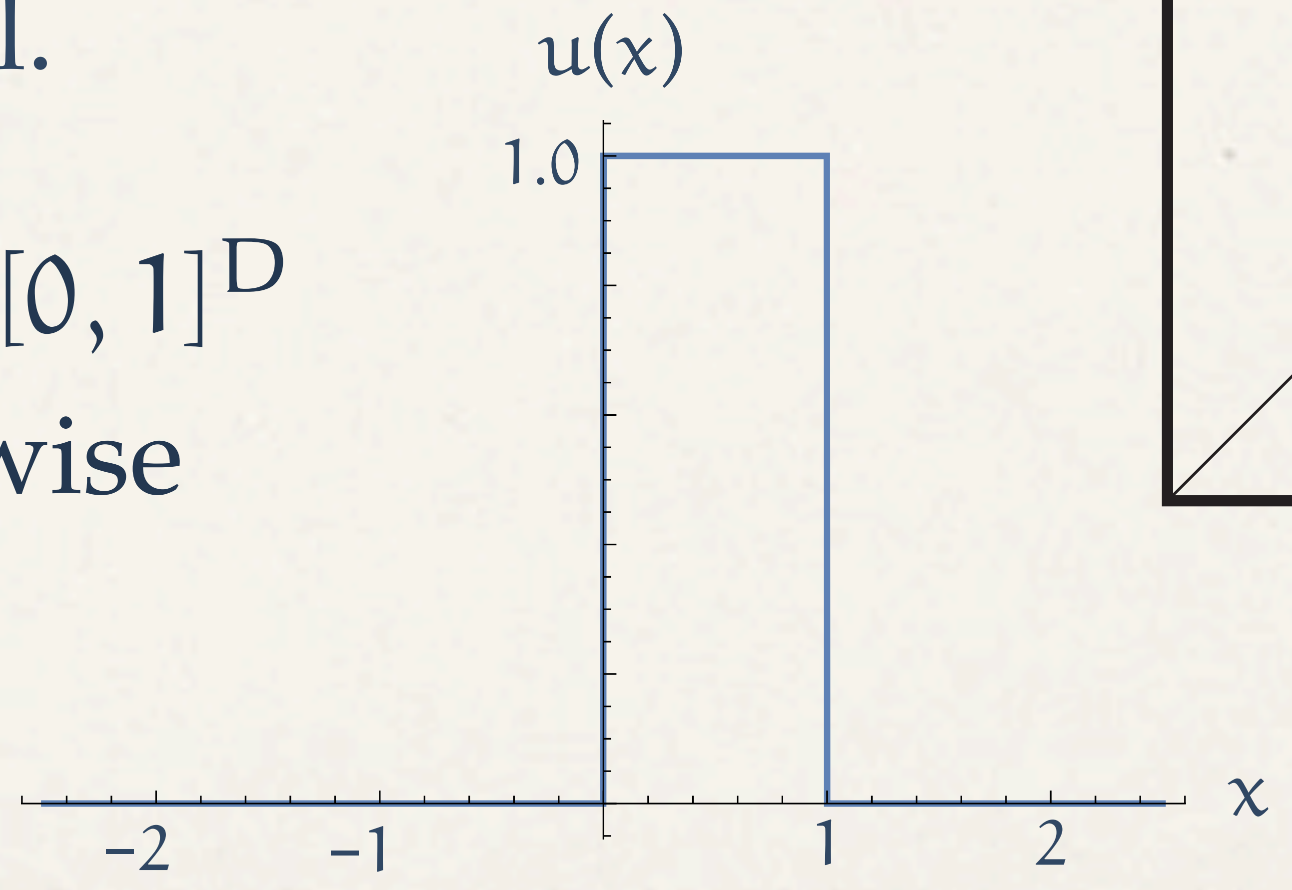
Given: a bounded function $f(\mathbf{x}) = f(x_1, \ldots, x_D)$ on the unit cube $[0,1]^D$ with $|f(\mathbf{x})| \leq 1$

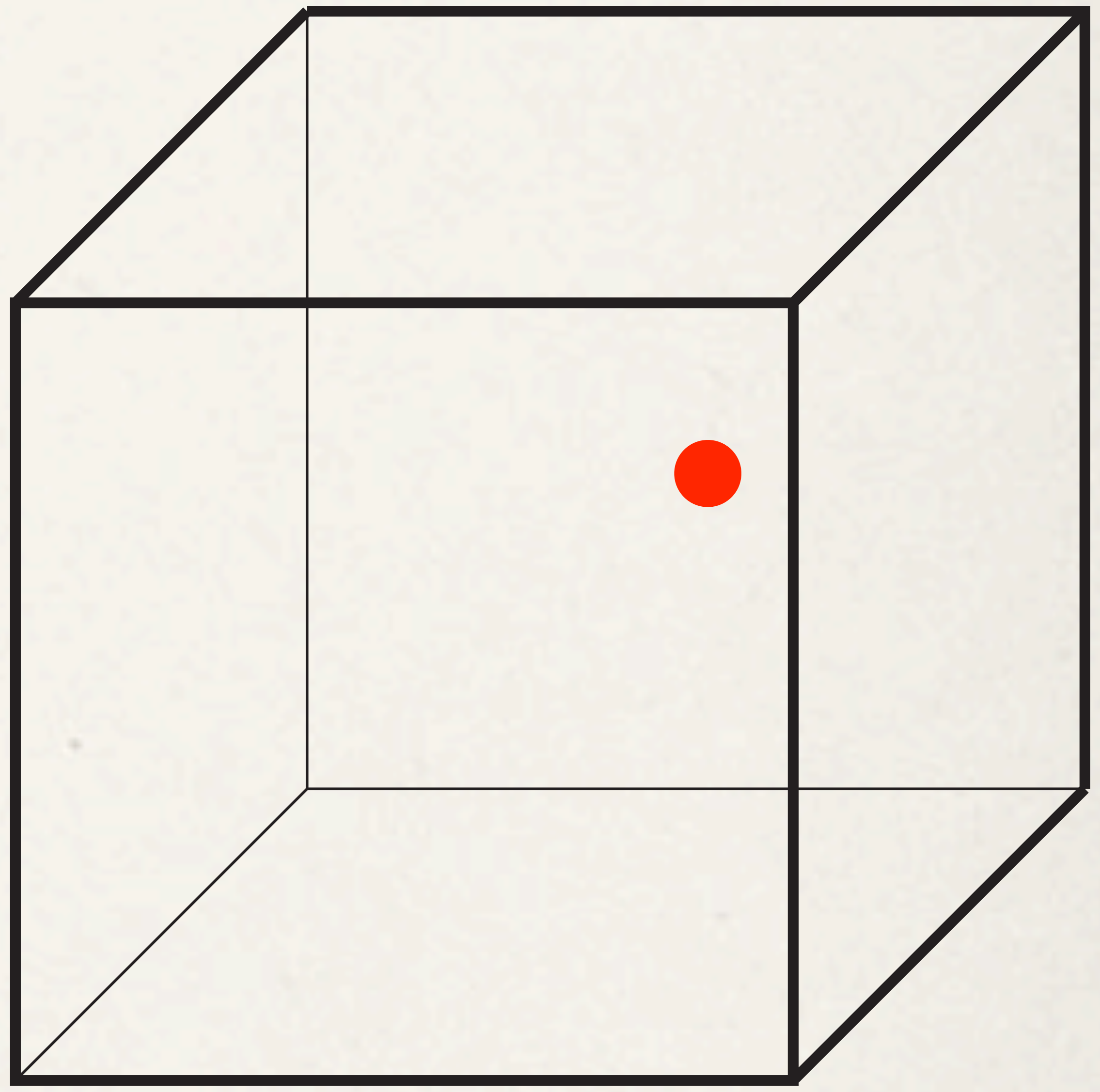
Compute: $J = \int \cdots \int_{[0,1]^D} f(\mathbf{x})\, d\mathbf{x}$

Select $\mathbf{X} = (X_1, \ldots, X_D)$ at random from the D-dimensional cube $[0, 1]^D$

This means: $X_1, \ldots, X_D$ are independent and are each uniformly distributed in the unit interval.

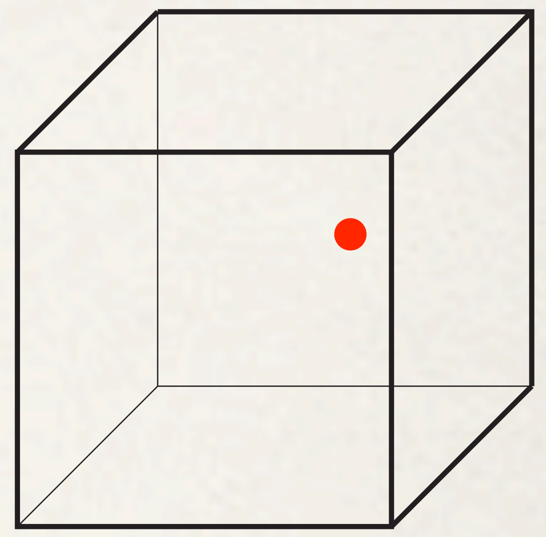
$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$





Evaluate $Y = f(\mathbf{X})$

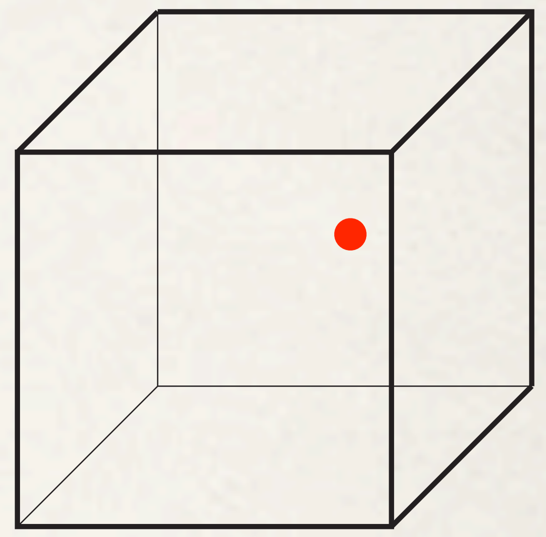
$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$



$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbb{E}\big(f(\mathbf{X})\big) = J$$

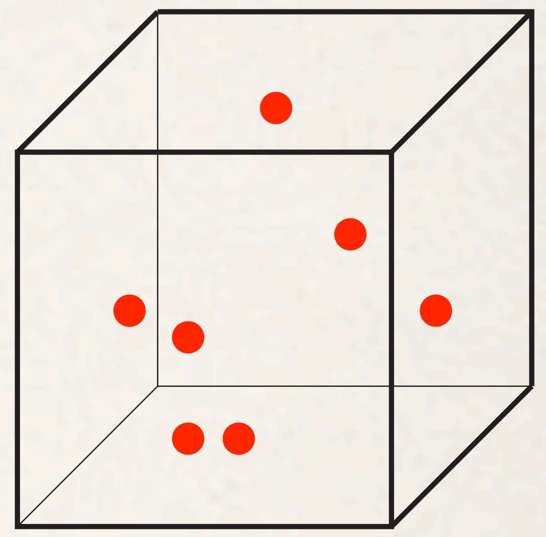
$$\mathrm{Var}\big(f(\mathbf{X})\big) \leq 1$$



$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbb{E}\big(f(\mathbf{X})\big) = J$$

$$\mathrm{Var}\big(f(\mathbf{X})\big) \leq 1$$

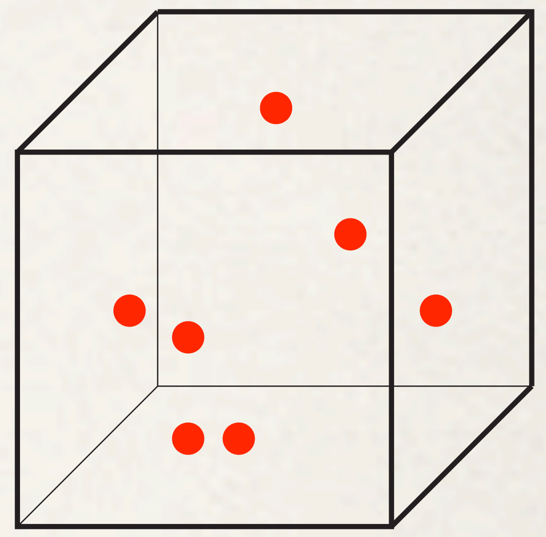


Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



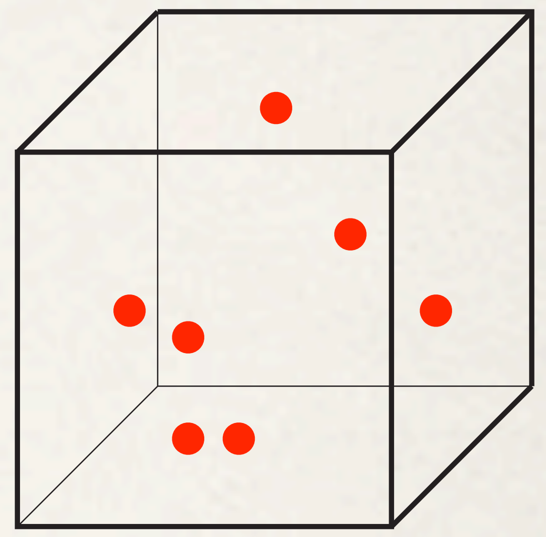
Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \ldots, Y_n = f(\mathbf{X}^{(n)})$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0,\ 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

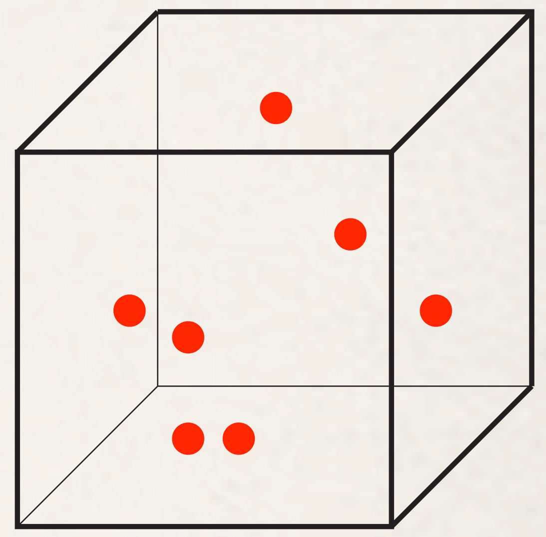
Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \ldots, Y_n = f(\mathbf{X}^{(n)})$

What do we know about these values?

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{E}(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \ldots, Y_n = f(\mathbf{X}^{(n)})$

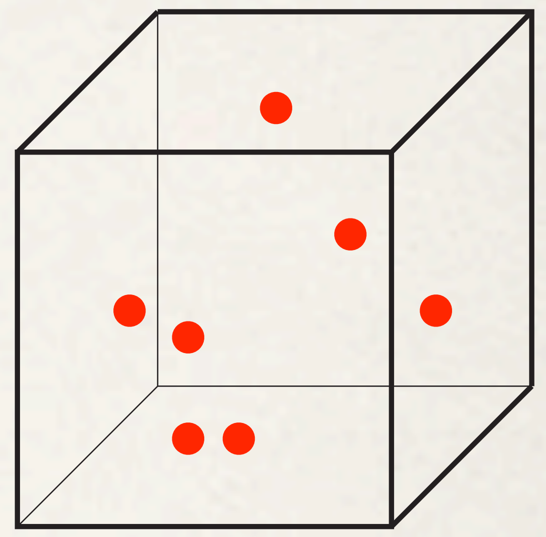
What do we know about these values?

The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E(f(\mathbf{X})) = J$$

$$\text{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \ldots, Y_n = f(\mathbf{X}^{(n)})$

What do we know about these values?

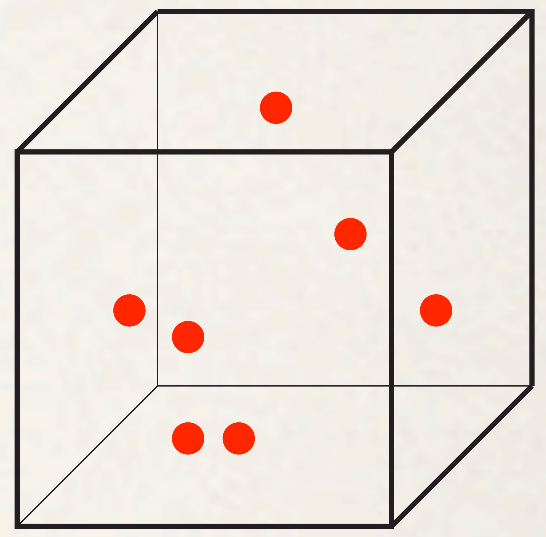
The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E\big(f(\mathbf{X})\big) = J$$

$$\mathrm{Var}\big(f(\mathbf{X})\big) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f\big(\mathbf{X}^{(1)}\big), Y_2 = f\big(\mathbf{X}^{(2)}\big), \ldots, Y_n = f\big(\mathbf{X}^{(n)}\big)$

What do we know about these values?

The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

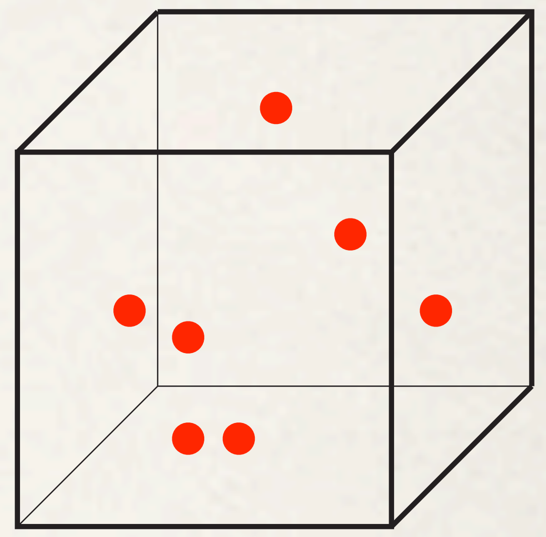
The law of large numbers beckons!

Form: $S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E\big(f(\mathbf{X})\big) = J$$

$$\operatorname{Var}\big(f(\mathbf{X})\big) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f\big(\mathbf{X}^{(1)}\big), Y_2 = f\big(\mathbf{X}^{(2)}\big), \ldots, Y_n = f\big(\mathbf{X}^{(n)}\big)$

What do we know about these values?

The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

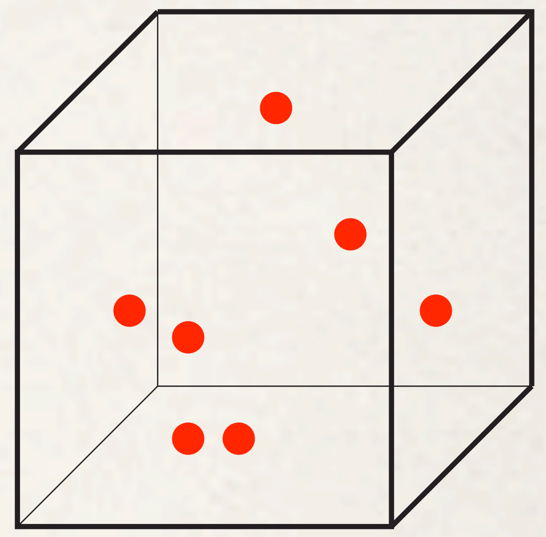
Form: $S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$

$E(S_n) = E(Y_1) + \cdots + E(Y_n)$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E\big(f(\mathbf{X})\big) = J$$

$$\operatorname{Var}\big(f(\mathbf{X})\big) \le 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f\big(\mathbf{X}^{(1)}\big), Y_2 = f\big(\mathbf{X}^{(2)}\big), \dots, Y_n = f\big(\mathbf{X}^{(n)}\big)$

What do we know about these values?

The induced sample $Y_1, \dots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

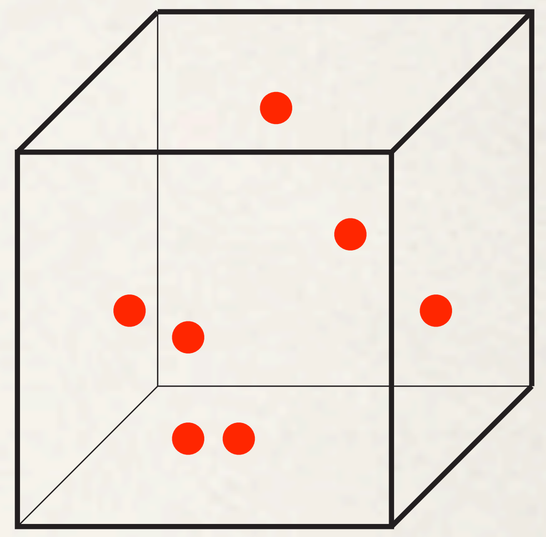
Form: $S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$

$$E(S_n) = E(Y_1) + \cdots + E(Y_n) = nJ$$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \dots, Y_n = f(\mathbf{X}^{(n)})$

What do we know about these values?

The induced sample $Y_1, \dots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

Form: $S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$

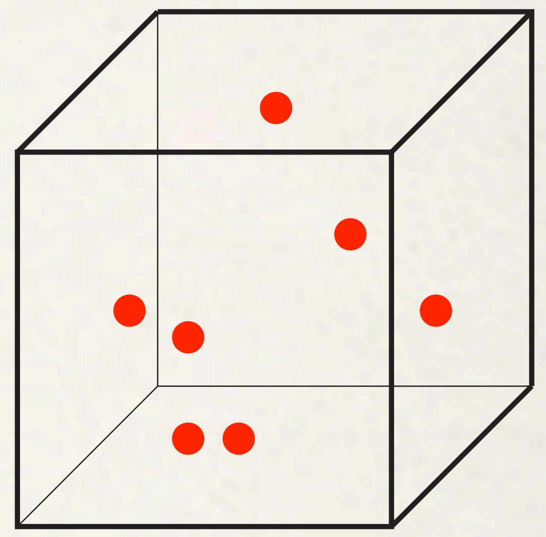
$$E(S_n) = E(Y_1) + \cdots + E(Y_n) = nJ$$

$$\mathrm{Var}(S_n) = \mathrm{Var}(Y_1) + \cdots + \mathrm{Var}(Y_n)$$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{E}\big(f(\mathbf{X})\big) = J$$

$$\mathrm{Var}\big(f(\mathbf{X})\big) \le 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f\big(\mathbf{X}^{(1)}\big), Y_2 = f\big(\mathbf{X}^{(2)}\big), \ldots, Y_n = f\big(\mathbf{X}^{(n)}\big)$

What do we know about these values?

The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

Form: $S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$

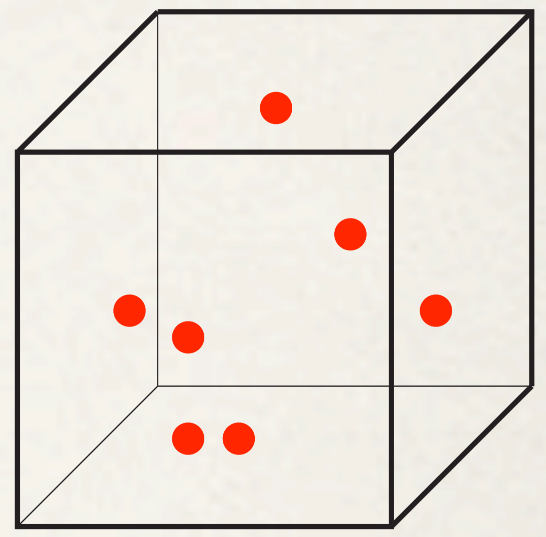
$$\mathbf{E}(S_n) = \mathbf{E}(Y_1) + \cdots + \mathbf{E}(Y_n) = nJ$$

$$\mathrm{Var}(S_n) = \mathrm{Var}(Y_1) + \cdots + \mathrm{Var}(Y_n) \le n \cdot 1 = n$$

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$E(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0,\ 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \dots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \dots, Y_n = f(\mathbf{X}^{(n)})$

What do we know about these values?

The induced sample $Y_1, \dots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

Form: $S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$

$$E(S_n) = E(Y_1) + \cdots + E(Y_n) = nJ$$

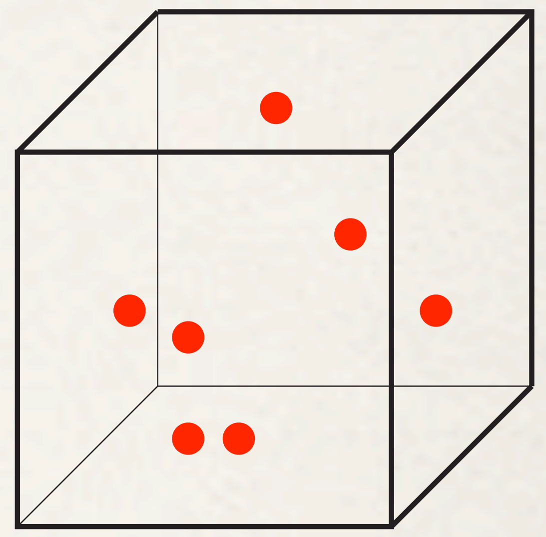
$$\mathrm{Var}(S_n) = \mathrm{Var}(Y_1) + \cdots + \mathrm{Var}(Y_n) \leq n \cdot 1 = n$$

Estimate the unknown J by the sample mean S_n/n

$$\mathbf{X} \sim p(\mathbf{x}) = u(x_1) \times \cdots \times u(x_D) = \begin{cases} 1 & \text{if } \mathbf{x} \in [0,1]^D \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{E}(f(\mathbf{X})) = J$$

$$\mathrm{Var}(f(\mathbf{X})) \leq 1$$



Generate an independent, random sample of points in the unit cube $[0, 1]^D$: $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots, \mathbf{X}^{(n)}$

Evaluate: $Y_1 = f(\mathbf{X}^{(1)}), Y_2 = f(\mathbf{X}^{(2)}), \ldots, Y_n = f(\mathbf{X}^{(n)})$

What do we know about these values?

The induced sample $Y_1, \ldots, Y_n$ constitutes a sequence of repeated independent trials with common expectation J and variance bounded above by 1.

The law of large numbers beckons!

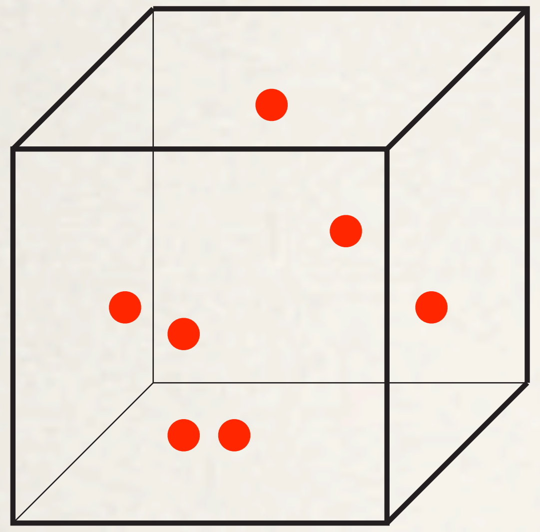
Form: $S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$

$$\mathbf{E}(S_n) = \mathbf{E}(Y_1) + \cdots + \mathbf{E}(Y_n) = nJ$$

$$\mathrm{Var}(S_n) = \mathrm{Var}(Y_1) + \cdots + \mathrm{Var}(Y_n) \leq n \cdot 1 = n$$

Monte Carlo method

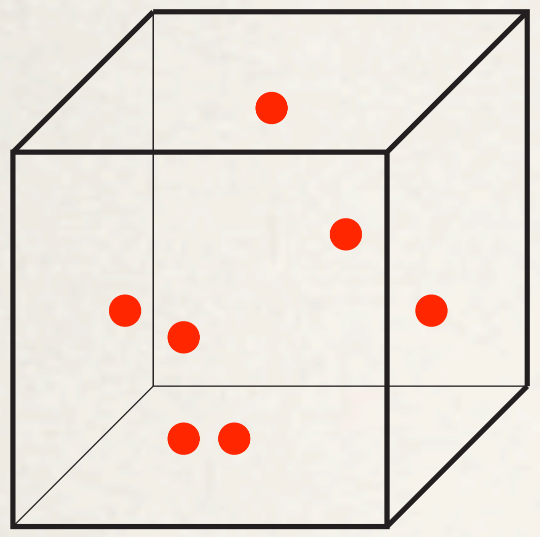
Estimate the unknown J by the sample mean S_n/n



$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \leq n$$

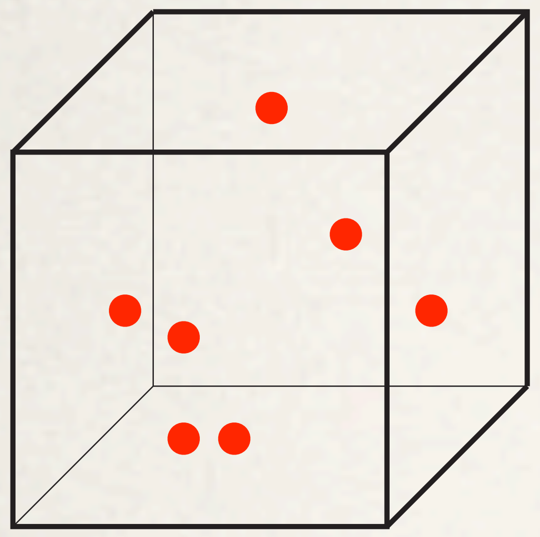


$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \le n$$

How well does the sample mean S_n/n estimate the unknown integral J?



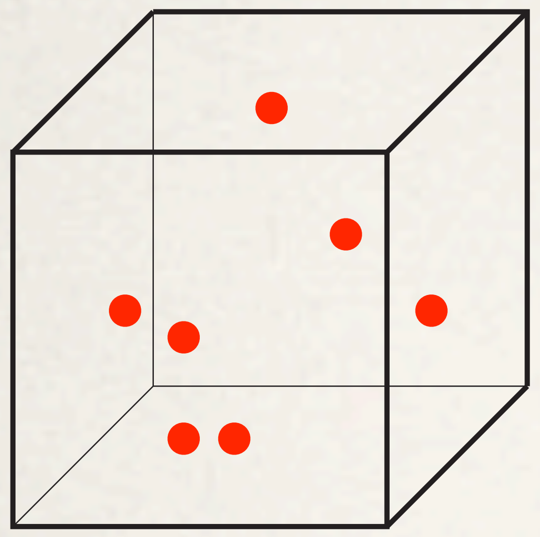
$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$\mathbf{E}(S_n) = nJ$$

$$\mathrm{Var}(S_n) \leq n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\}$$



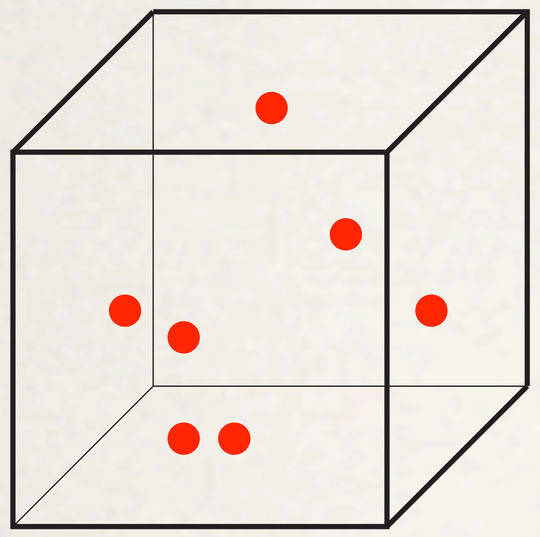
$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$\mathbf{E}(S_n) = nJ$$

$$\mathrm{Var}(S_n) \leq n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\}$$



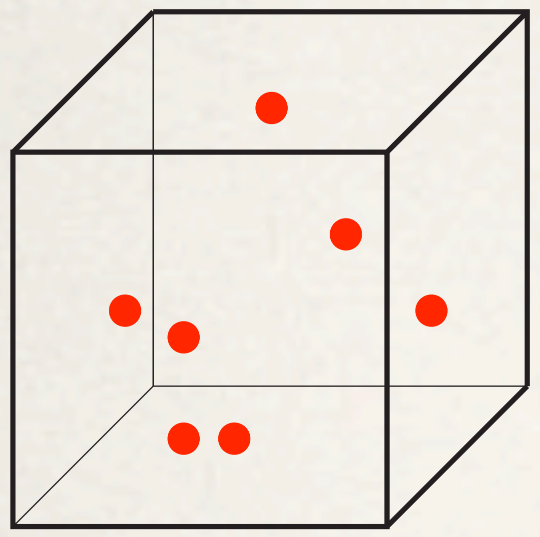
$$S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \leq n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\} \leq \frac{\mathrm{Var}\, S_n}{(n\epsilon)^2}$$



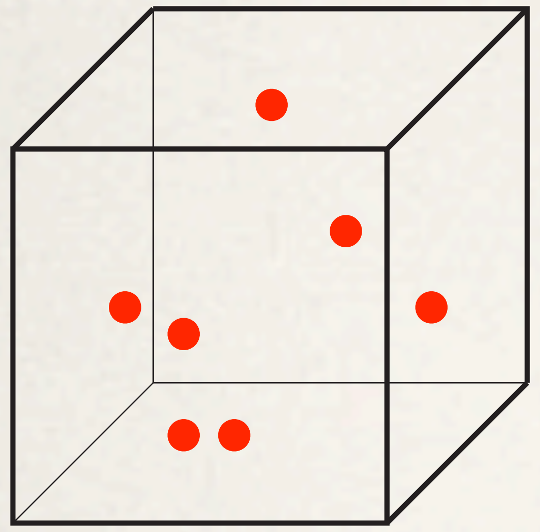
$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \le n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\} \le \frac{\mathrm{Var}\, S_n}{(n\epsilon)^2} \le \frac{n}{n^2\epsilon^2}$$



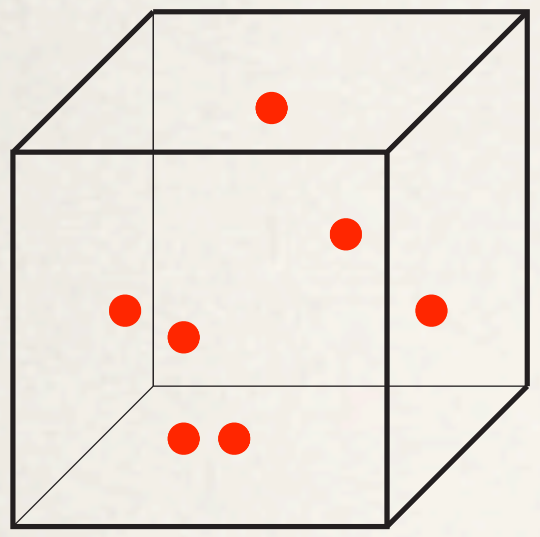
$$S_n = Y_1 + \cdots + Y_n = f\big(\mathbf{X}^{(1)}\big) + \cdots + f\big(\mathbf{X}^{(n)}\big)$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \le n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\} \le \frac{\mathrm{Var}\, S_n}{(n\epsilon)^2} \le \frac{n}{n^2\epsilon^2} = \frac{1}{n\epsilon^2}$$



$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$E(S_n) = nJ$$

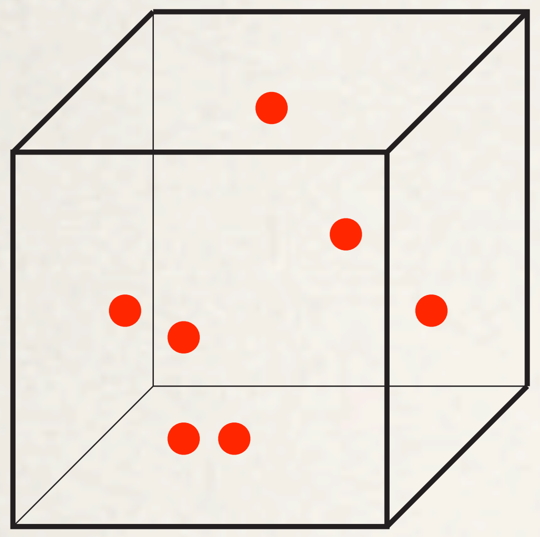
$$\mathrm{Var}(S_n) \le n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\} \le \frac{\mathrm{Var}\, S_n}{(n\epsilon)^2} \le \frac{n}{n^2\epsilon^2} = \frac{1}{n\epsilon^2}$$

The sample mean S_n/n estimate the unknown integral J with an absolute error of no more than ϵ and a confidence of at least $1 - \delta$ if the sample size n satisfies

$$\frac{1}{n\epsilon^2} \le \delta \qquad \text{—or—} \qquad n \ge \frac{1}{\epsilon^2\delta}$$



$$S_n = Y_1 + \cdots + Y_n = f(\mathbf{X}^{(1)}) + \cdots + f(\mathbf{X}^{(n)})$$

$$E(S_n) = nJ$$

$$\mathrm{Var}(S_n) \le n$$

How well does the sample mean S_n/n estimate the unknown integral J?

$$\mathbf{P}\left\{\left|\frac{S_n}{n} - J\right| > \epsilon\right\} = \mathbf{P}\{|S_n - nJ| > n\epsilon\} \le \frac{\mathrm{Var}\, S_n}{(n\epsilon)^2} \le \frac{n}{n^2\epsilon^2} = \frac{1}{n\epsilon^2}$$

The sample mean S_n/n estimate the unknown integral J with an absolute error of no more than ϵ and a confidence of at least $1 - \delta$ if the sample size n satisfies

$$\frac{1}{n\epsilon^2} \le \delta \qquad \text{—or—} \qquad n \ge \frac{1}{\epsilon^2\delta}$$

To illustrate: if $n = 10^6$ then the estimate error will be less than 1% ($\epsilon = 0.01$) and the confidence in excess of 99% ($\delta = 0.01$)!