# Monte Carlo Integration Error Analysis

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## Abstract:
This work deals with Monte Carlo integration error analysis problem.. The main result is that the Monte Carlo integration error is proportional to $n^{-1/2}$, and the *n* dependence of the error is independent of the nature of the integrand and, most importantly, independent of the number of dimensions This work also presents the analytical derivation of the relation $\sigma/\sqrt{n}$ in addition to the error estimate for numerical integration methods.

## 1. Introduction
Both the classical numerical integration methods and the Monte Carlo methods yield approximate answers whose accuracy depends on the number of intervals or on the number of trials respectively [2], [4]. So far, we have used the exact value of various integrals to determine the error in the Monte Carlo method approaches zero as approximately $n^{-1/2}$ for large number of trials *n* this is due to the central limit theorem [9]. Section 2 discussed how to estimate the Monte Carlo error, while section 3 estimates the error of the numerical integration methods [10]. Finally section 4 shows the analytical derivation of the standard deviation of the mean [10].

## 2. Monte Carlo Error Estimating
In the following, we shall find how to estimate the error when the exact solution is unknown. Our main result is that the *n* dependence of the error is independent of the nature of the integrand and, most importantly, independent of the number of dimensions [9].

Because the appropriate measure of the error in Monte Carlo calculations is subtle [10], we first determine the error for an explicit example. Consider the Monte Carlo evaluation of the integral of $f(x)=\sqrt{x}$ in the interval [0, 4]. Our result for a particular sequence of $n=10^5$ random number using the sample mean method is $F_n = 5.332517$ . By comparing $F_n$ to the exact result of $F = 5.333333$, we find that the error associated with $n=10^5$ trials is approximately 0.000817.

The best way to estimate the error if the exact result is unknown, so to calculate the probability that the true value $F$ is within a certain range centered on $F_n$ .If the integrand is constant, then the error would be zero, that is, $F_n$ would equal $F$ for any *n*. This limiting behavior suggests that a possible measure of the error is the variance $\sigma^2$ defined by [6], [7],[10]:

$$\sigma^2 = \langle f^2 \rangle - \langle f \rangle^2 \qquad (1)$$

Where

$$\langle f \rangle = \frac{1}{n}\sum_{i=1}^{n} f(x_i) \qquad (2.a)$$

$$\langle f^2 \rangle = \frac{1}{n}\sum_{i=1}^{n} f(x_i)^2 \qquad (2.b)$$

From the definition of the standard deviation $\sigma$ , we see that if *f* is independent of *x*, $\sigma$ is zero. For our example and the same sequence of random numbers used to obtain $F_n = 5.332517$, we obtain $\sigma_n = 0.00742$. Because this value of $\sigma$ is two larger than the actual error, we conclude that $\sigma$ cannot be a direct measure of this error. Instead $\sigma$ is a measure of how much the function *f(x)* varies in the interval of interest.

Another clue to finding an appropriate measure of the error can be found by increasing *n* and seeing how the actual error decreases as *n* increase [9], [10]. In table 1 we see that as *n* goes from $n=10$ to $n=10^5$, the actual error decreases by a factor of 10, that is, as $\approx 1/n^{1/2}$. However, we also see that $\sigma_n$ is roughly constant and is much larger than the absolute error $|F_n - F|$.

| *n* | $F_n$ | $\lvert F_n - F\rvert$ | $\sigma_n$ |
|---|---|---|---|
| 10 | 5.192817 | 0.140517 | 0.229488 |
| $10^2$ | 5.517878 | 0.184545 | 0.151467 |
| $10^3$ | 5.394788 | 0.061454 | 0.034668 |
| $10^4$ | 5.306105 | 0.027229 | 0.041050 |
| $10^5$ | 5.332517 | 0.000817 | 0.007420 |

Table 1: Examples of Monte Carlo measurements of the mean value of $f(x)=\sqrt{x}$ in the interval [0, 4]. The standard deviation $\sigma_n$ is found using (1)

One way to obtain an estimate for the error is to make additional runs of *n* trails. Each runs of *n* trials yields a mean or measurement which is denoted by $M_\alpha$ . In general, these measurements are not equivalent because each of which use a different finite sequence of random numbers [10]. Table 2 shows the results of ten separate measurements of $n=10^5$ trials each.

| Run $\alpha$ | $M_\alpha$ | $\lvert M_\alpha - F\rvert$ |
|---|---|---|
| 1 | 5.327045 | 0.006288 |
| 2 | 5.340285 | 0.006952 |
| 3 | 5.326770 | 0.006563 |
| 4 | 5.323363 | 0.009970 |
| 5 | 5.324491 | 0.008842 |
| 6 | 5.310109 | 0.023225 |
| 7 | 5.350355 | 0.017021 |
| 8 | 5.368457 | 0.035124 |
| 9 | 5.308147 | 0.025186 |

| | | |
|---|---|---|
| 10 | 5.341014 | 0.007681 |

Table 2: Examples of Monte Carlo measurements of the mean value of $f(x)=\sqrt{x}$ in the interval [0, 4]. A total of 10 measurements of $n=10^5$ trials each were made. The mean value $M_\alpha$ and the absolute error for each measurement are shown.

From table 2 we see that the absolute error varies from measurement to another. Qualitatively, the magnitude of the difference between the measurements is similar to the actual errors, and hence these differences are a measure of the error associated with a single measurement. To obtain a quantitative measure of this error, we determine the differences of these measurements using the standard deviation of the means $\sigma_m$ which is defined as [7], [9], [10]:

$$\sigma_m{}^2 = \langle M^2\rangle - \langle M\rangle^2 \quad (3)$$

Where

$$\langle M\rangle = \frac{1}{m}\sum_{\alpha=1}^{m} M_\alpha \quad (4.a)$$

$$\langle M^2\rangle = \frac{1}{m}\sum_{\alpha=1}^{m} M^2{}_\alpha \quad (4.b)$$

From the values of $M_\alpha$ in table 2 and the relation (3), we find that $\sigma_m = 0.01746$. This value of $\sigma_m$ is consistent with the results for the absolute errors shown in table 2 which varies from 0.006288 to 0.035124. Hence we conclude that $\sigma_m$ is a measure of the error for a single measurement. The more precise interpretation of $\sigma_m$ is that a single measurement has a 99.88% chance of being within $\sigma_m$ of the true mean. Hence the probable error associated with $\sigma_m$ for first measurement of $F_n$ with $n=10^5$ is $5.327045 \mp 0.006288$.

Although $\sigma_m$ gives an estimate of the probable error , our method of obtaining $\sigma_m$ by making additional measurements is impractical because we could have combining the additional measurements to make a better estimate. In section 4 we derive the relation [10]

$$\sigma_m = \frac{\sigma}{\sqrt{n-1}} \quad (5.a)$$

$$\approx \frac{\sigma}{\sqrt{n}} \quad (5.b)$$

The reason for the expression $1/\sqrt{n-1}$ in (5.a) rather than $1/\sqrt{n}$ is similar to the reason for the expression $1/\sqrt{n-2}$ in the error estimates of the least squares fits [5], [10]. To compute $\sigma$, we need to use *n* trials to compute the mean $\langle f(x)\rangle$ and we have only (*n-1*) independent trials remaining to calculate $\sigma$. Because we almost always make a large number of trials , we will use the relation (5.b) and consider only this limit in section 3. From (5) the probable error of our initial measurement is approximately 0.00742/316.228 ≈ 0.000024, which is consistent with the known error of 0.0008177 and with our estimated value of $\sigma_m \approx 0.01746$.

One way to verify the relation (5) is to divide the initial measurement of *n* trials into *s* subsets. This procedure does not require additional measurements. We denote the mean value of $f(x_i)$ in the *kth* subset by $S_k$ [9], [10]. As an example, we divide the $10^5$ trials of the first measurement into *s* = 10 subsets of $n/s = 10^4$ trials each. The results for $S_k$ are shown in table 3.

| Subset *k* | $S_k$ | $\lvert S_k - F\rvert$ |
|---|---|---|
| 1 | 5.539686 | 0.026352 |
| 2 | 5.344153 | 0.010819 |
| 3 | 5.357490 | 0.024156 |
| 4 | 5.371903 | 0.038569 |
| 5 | 5.305586 | 0.027747 |
| 6 | 5.327480 | 0.005853 |
| 7 | 5.325547 | 0.007786 |
| 8 | 5.347085 | 0.013752 |
| 9 | 5.313694 | 0.019640 |
| 10 | 5.344287 | 0.010954 |

Table 3: The values of $S_k$ for $f(x)=\sqrt{x}$ for $0 \le x \le 4$ is shown for 10 subsets of $10^4$ trials each. The average value of *f(x)* over the 10 subsets is 5.33969, agree with the result of $F_n$ for the first measurement shown in table 2.

As expected, the mean value of *f(x)* for each subset *k* do not equal. A reasonable candidate for a measure of the error is the standard deviation of the means $\sigma_s$ of each subset, where

$$\sigma_s{}^2 = \langle S^2\rangle - \langle S\rangle^2 \quad (6)$$

where the average are over the subsets [10]. From table 3 we obtain $\sigma_s = 0.0201$, a result that is approximately equal to our estimate of 0.01746 for $\sigma_m$. However, we would like to define an error estimate that is independent of how we subdivide the data. This quantity is not $\sigma_s$, but the ratio $\sigma_s/\sqrt{s}$ which for our example is approximately $0.0201/\sqrt{10} \approx 0.0064$. This value is consistent with both $\sigma_m$ and the ratio $\sigma/\sqrt{n}$. We conclude that we can interpret the *n* trials either as a single measurement or as a collection of s measurements with *n/s* trials each. In the former interpretation the probable error is given by the standard deviation of the *n* trials divided by the square root of the number of trials. In the same spirit, the later interpretation implies that the probable error is given by the standard deviation of the *s* measurements of the subsets divided by the square root of the number of measurements [10].

## 3. Error Estimates for Numerical Integration

The truncation error estimates is depended on the number of intervals for the numerical integration methods. These estimates are based on the assumed adequacy of the Taylor series expansion of the integrand *f(x)* [1], [10]:

$$f(x)=f(x_i)+f'(x_i)(x-x_i)+\tfrac{1}{2}f''(x_i)(x-x_i)^2+\dots \quad (7)$$

and the integration of (1) in the interval $x_i \le x \le x_{i+1}$

$$\int_{x_i}^{x_{i+1}} f(x)dx = f(x_i)\Delta x+\tfrac{1}{2}f'(x_i)(\Delta x)^2+\tfrac{1}{6}f''(x_i)(\Delta x)^3+\cdots$$

(8)

We first estimate the error associated with the rectangular methods with *f(x)* evaluated at the left side of each interval. Let error $\Delta_i$ in the interval $[x_i, x_{i+1}]$ be the difference between (8) and the estimate $f(x_i)\Delta x$:

$$\Delta_i = \int_{x_i}^{x_{i+1}} f(x)dx - f(x_i)\Delta x \approx \tfrac{1}{2}f'(x_i)(\Delta x)^2 \quad (9)$$

We see that to leading order in $\Delta x$ the error in each interval is of order $(\Delta x)^2$. Because there are a total of *n* intervals and $\Delta x=(b-a)/n$, the total error associated with the rectangular methods is

$$n\Delta_i \approx n(\Delta x)^2 \approx n^{-1}.$$

The estimated error associated with the trapezoidal rule can be found in the same way [3],. The error in the interval $[x_i, x_{i+1}]$ is the difference between the exact integral and the estimated one:

$$\tfrac{1}{2}[f(x_i)+f(x_{i+1})]\Delta x$$

$$\Delta_i = \int_{x_i}^{x_{i+1}} f(x)dx - \tfrac{1}{2}[f(x_i)+f(x_{i+1})]\Delta x \quad (10)$$

If we use (8) to estimate the integral and (7) to estimate $f(x_{i+1})$ in (10), we find that the term proportional to the first derivative $f'$ cancels and that the error associated with one interval is of order $(\Delta x)^3$. Hence, the total error in the interval [*a*, *b*] associated with the trapezoidal rule is of order $n^{-2}$ [10].

Because Simpson's rule is based on fitting *f(x)* in the interval $[x_i, x_{i+1}]$ to a parabola, error terms proportional to $f''$ is omitted. We might expect that error terms of order $f'''(x_i)(\Delta x)^4$ contribute, but these terms canceled by virtue of their symmetry. Hence the $(\Delta x)^4$ term of the Taylor expansion of *f(x)* is adequately represented by Simpson's rule.If we retain the $(\Delta x)^4$ term in the Taylor series of *f(x)* we find that the error in the interval $[x_i, x_{i+1}]$ is of order $f''''(x_i)(\Delta x)^5$ and the total error in the interval [*a*, *b*] associated with Simpson rule is of order $O(n^{-4})$.

The error estimates can be extended to two dimensions in a similar manner [2]. The two dimensional integral of *f(x, y)* is the volume under the surface determined by *f(x, y)*. In the rectangular approximation methods, the integral is written as a sum of the volumes of parallelograms with cross sectional area $\Delta x\Delta y$ and a height determined by *f(x, y)* at one side. To determine the error we expand *f(x, y)* in a Taylor series [1], [3], [10]

$$f(x,y)=f(x_i,y_i)+\frac{\partial f(x_i,y_i)}{\partial x}(x-x_i)+\frac{\partial f(x_i,y_i)}{\partial y}(y-y_i)+\cdots$$

(11)

and write the error as

$$\Delta_i = \iint f(x,y)dxdy - f(x_i,y_i)\Delta x\Delta y \quad (12)$$

If we substitute (11) in (12) and integrate each term, we find that the term proportional to *f* and the integral of *(x - x<sub>i</sub>) dx* yields $\tfrac{1}{2}(\Delta x)^2$. The integral of this term with respect to *dy* gives another factor of $\Delta y$. The integral of the term proportional to $(y-y_i)$ yield a similar contribution. Because $\Delta y$ also is order $\Delta x$, the error associated with the interval $[x_i, x_{i+1}]$ and $[y_i, y_{i+1}]$ is of leading order in $\Delta x$:

$$\Delta_i \approx \tfrac{1}{2}[f'_x(x_i,y_i)+f'_y(x_i,y_i)](\Delta x)^3 \quad (13)$$

We see that the error associated with one parallelogram is of order $(\Delta x)^3$. Because there are *n* parallelograms, the total error is order $n(\Delta x)^3$. However, in two dimensions the total error is of order $n^{-1/2}$. In contrast the total error in one dimension is order $n^{-1}$ as we saw earlier.

The corresponding error estimates for the two dimensional generalizations of the trapezoidal rule and Simpson's rule are of order $n^{-1}$ and $n^{-2}$ respectively. In general if the error goes as of order $n^{-a}$ in one dimension then the error in *d* dimensions goes as $n^{-a/d}$ .In contrast Monte Carlo errors vary as of order $n^{-1/2}$ independent of *d*. Hence for large enough dimension *d*, Monte Carlo
integration method will lead to smaller errors for the same choice of *n* [9], [10].

## 4. The Standard Deviation of the Mean

In section 2 we gave empirical reasons for the claim that the error associated with a single measurement consisting of *n* trials equals $\sigma/\sqrt{n}$, where $\sigma$ the standard deviation in a single is measurement. We now present an analytical derivation of this relation [7], [8], [10].

The quantity of experimental interest is denoted as *x*. Consider *m* sets of measurements each with *n* trials for total *mn* trials. We use the index $\alpha$ to denote a particular measurement and the index *i* to designate the *ith* trial within a measurement. We denote $x_{\alpha,i}$ as trial *i* in the measurement $\alpha$. The value of a measurement is given by [7], [8], [10]:

$$M_\alpha = \tfrac{1}{n}\sum_{i=1}^{n} x_{\alpha,i} \quad (14)$$

The mean $\overline{M}$ of the total mn individual trials is given by

$$\overline{M}=\frac{1}{m}\sum_{\alpha=1}^{m}M_\alpha=\frac{1}{nm}\sum_{\alpha=1}^{m}\sum_{i=1}^{n}x_{\alpha,i} \quad (15)$$

The difference between measurement $\alpha$ and the mean of all the measurements is given by

$$e_\alpha = M_\alpha - \overline{M} \quad (16)$$

We can write the variance of the means as

$$\sigma_m^2 = \tfrac{1}{m}\sum_{\alpha=1}^{m} e_\alpha^2 \qquad (17)$$

Now we wish to relate $\sigma_m$ to the variance of the individual trials. The discrepancy $d_{\alpha,i}$ between an individual sample $x_{\alpha,i}$ and the mean is given by [3], [10]:

$$d_{\alpha,i} = x_{\alpha,i} - \overline{M} \qquad (18)$$

Hence the variance $\sigma^2$ of the $mn$ individual trials is

$$\sigma^2 = \frac{1}{mn}\sum_{\alpha=1}^{m}\sum_{i=1}^{n} d_{\alpha,i}{}^2 \qquad (19)$$

whence

$$e_\alpha = M_\alpha - \overline{M} = \frac{1}{n}\sum_{i=1}^{n}(x_{\alpha,i} - \overline{M}) \qquad (20)$$

$$= \frac{1}{n}\sum_{i=1}^{n} d_{\alpha,i} \qquad (21)$$

If we substitute (21) into (17) we get

$$\sigma_m^2 = \frac{1}{m}\sum_{\alpha=1}^{n}\left(\tfrac{1}{n}\sum_{i=1}^{n} d_{\alpha,i}\right)\left(\tfrac{1}{n}\sum_{j=1}^{n} d_{\alpha,j}\right) \qquad (22)$$

The sum in (22) over trials *i* and *j* in set $\alpha$ contains two kinds of terms those with *i* = *j* and those with $i \neq j$ . We expect that $d_{\alpha,i}$ and $d_{\alpha,j}$ are independent and equally positive or negative on the average. Hence in the limit of a large number of measurements we expect that only the terms with *i* = *j* in (22) will survive and we write

$$\sigma_m^2 = \frac{1}{mn^2}\sum_{\alpha=1}^{n}\sum_{i=1}^{n} d_{\alpha,i}^2 \qquad (23)$$

If we combine (23) with (19) we arrive at the desired result [10]

$$\sigma_m^2 = \frac{\sigma^2}{n} \qquad (24)$$

## Reference:


1. Burden, Richard L., Faires, J. Douglas and Reynolds, Albert G, Numerical Analysis, Prindle, Weber and Schmidt, 7th Edition, 2001.
2. Don Ferguson , Numerical integration , Survey Report, Academic Press, New York. 2002.
3. Davis, Philip J. and Rabinowitz, Philip, Methods of Numerical Integration**,** Academic Press, Inc.,1975.
4. Judd, Kenneth L., Numerical Methods in Economic**,** Springer-Verlag, New York, 1998.
5. Keller, Gerald and Warrack Brian, Statistics for Management and Economics , Thomson Learning, Inc., 6th Edition, 2003.
6. Malvin H. Kalos and Paula A. Whitlock, Monte Carlo Methods, vol. 1: Basics, John Wiley & Sons, 1986.
7. Press W. H., Teukolsky, S. A., Vetterling, W. H. and Flannery, B. P., Numerical Recipes in C , Cambridge University Press, 2nd Edition, 1992.
8. Reuven Y. Rubinstein, Simulation and the Monte Carlo Method, John Wiley & Sons, 1981.
9. Sabelfeld, K. K. , Monte Carlo methods and applications , John Wiley & Sons, Vol. 10, 2004.
10. http://physics.clarku.edu/couses/125/gtcdraft/chapter11.pdf.

# تحليل خطأ تكامل مونت كارلو

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**الملخص**

تناول هذا البحث مسألة تحليل خطأ تكامل مونت كارلو. النتيجة الرئيسة في هذا البحث هي أن خطأ .
تكامل مونت كارلو يتناسب مع $n^{-1/2}$ . وأنه لا يعتمد على طبيعة الدالة المراد تكاملها ولا يعتمد على عدد أبعاد التكامل.
استعرض البحث أيضا الاشتقاق التحليلي للعلاقة $\sigma / \sqrt{n}$ إضافة إلى تقدير خطأ طرائق التكامل العددي.