積分ルーチンDICEにおける負相関変量の導入

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Introduction of antithetic variates to integration routine DICE

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Abstract

自動積分ルーチンDICEの積分推定量に負相関変量を導入した。新しい推定量は被積分関数が滑らかな関数であるときに効果があり、分割された小領域においてランダムサンプルする際のサンプル点の個数が小さい方がこの積分法の総サンプル点数を減じる上で有効であることが判明した。

Antithetic variates are introduced in the integral estimator of automatic integration routine DICE. The new estimator is found to be effective when the integrand is smooth function and the smaller the number of sample points randomly sampled in the divided small region is effective in reducing the total number of sample points for the integration.

Keywords: Antithetic Variates, Automatic Integration, Monte Carlo method

1 Introduction

One of important matters of numerical integration is efficient sampling. In a previous paper[9] I have reported the present status of integration routine DICE which estimates the value of the definite integral whose integrand is not only smooth function but also has such singularity that a range of very sharp peaks with very narrow width lies in the integral region. Such kind of integrand appears in the phase space integral of scattering processes of elementary particle physics. Numerical integration to estimate multi-dimensional definite integrals with such singularities is never easy and always fails to obtain credible results without use of any transformation of integral variables to remove them or at least to diminish them at all.

One of targets to develop integration routine DICE is to compute such difficult definite integrals automatically and get somehow credible estimates of them. However it requires a large number of sample points to estimate the integral of which integrand has very sharp peaks with very narrow width. The method of integration requires further much more sample points when dimension of integral becomes higher.

It is important to study efficient sampling method in order to reduce sampling points required to obtain an estimate of integral within a given accuracy. DICE uses both of two sampling methods, fixed sampling and random sampling. The random sampling would be considered as one of possibilities to improve the efficiency.

In Monte Carlo method the major problem is how to reduce the variance of an estimate of some quantity θ to study in the simulation. In the chapter of general principles of the Monte Carlo method of Ref.[2] the relative efficiency of two Monte Carlo methods, the efficiency of method 2 relative to method 1, is given by the following expression:

$$\frac{n_1\sigma_1^2}{n_2\sigma_2^2}$$

where n_1 and n_2 are required units of computing time and σ_1^2 and σ_2^2 are the variances of estimates of θ in two method 1 and 2, respectively. Thus reduction of variance is identical with improvement in effciency of

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the Monte Carlo method. Use of antithetic variables is one of several methods of variance reduction shown in the textbook[8].

The name of antithetic variates was introduced in 1956 by Hammersley and Morton[1]. In the classical papers of numerical integration[3, 4] Haber proposed a modified Monte-Carlo quadrature method to get more accurate estimates of integrals than those would be obtained by simple Monte Carlo method. He applied antithetic variates to the estimator of a very simple case of stratified sampling.

In this paper we introduce antithetic variates in the estimator of integral for random sampling in the routine DICE v1.3[7]. We report the results of using antithetic variates in the integral estimator in comparison with those of the usual integral estimator in the Monte Carlo method.

2 Implementation

Dividing rule of integral region is briefly explained[6]. Let us consider first in 2 dimension. The integral plane is divided into 2×2 equal sized subregions. Similarly in N dimension the integral region is divided into 2^N equal sized subregions. In each subregion a series of division condition tests with using regular sampling[7] and random sampling are performed in order, to decide whether divide it further into 2^N subregions or not.

These sampling tests are made repeatedly such that singular part of the integral region can be finely divided. We define the level of division `L` and the first level is `L=1` and the second level of division is `L=2` and so on. After repeating the sampling test finally the division condition does not hold at some level of division or the level of division reaches to the limit value `L=LIMIT`. DICE keeps the maximum level of division `Lmax` of each iteration as output data.

When division condition does not hold the integral estimate $\hat{I}_i$ and the variance estimate $\hat{\sigma_i}^2$ of subregion i are evaluated. The usual integral estimator of random sampling for subregion i is written by

$$\hat{I}_i = \frac{\Delta_i}{\texttt{NSAMPL}} \sum_{k=1}^{\texttt{NSAMPL}} f(\mathbf{x}_k^{(i)}) \ , \qquad (1)$$

where Δ_i is volume of subregion i. `NSAMPL` is number of calls to estimate the integrand function f at the points with rectangular coordinates $\mathbf{x}_k^{(i)}, k = 1, 2, \cdots, \texttt{NSAMPL}$ in subregion i. The coordinate $\mathbf{x}_k^{(i)}$ is randomly taken and uniformly distributed in subregion i.

The new integral estimator of subregion i uses the antithetic variates is denoted by the subscript $_{AV}$ and given by

$$\hat{I}_{i,AV} = \frac{\Delta_i}{\texttt{NSAMPL}} \sum_{k=1}^{\texttt{NSAMPL}} \frac{f(\mathbf{x}_k^{(i)}) + f(\mathbf{x}_k^{(i)*})}{2} \ . \qquad (2)$$

Both $\mathbf{x}_k^{(i)}$ and $\mathbf{x}_k^{(i)*}$ are rectangular coordinates. $\mathbf{x}_k^{(i)}$ is randomly taken and uniformly distributed in subregion i. However $\mathbf{x}_k^{(i)*}$ is taken as symmetrically opposite to $\mathbf{x}_k^{(i)}$ within subregion i.

Now we have two estimators of integral $\hat{I}$ and $\hat{I}_{AV}$ whose variances are denoted by $var(\hat{I})$ and $var(\hat{I}_{AV})$. The subscript $_{AV}$ indicates use of antithetic variates. The expressions are given by

$$\left.\begin{array}{rcl} \hat{I} & = & \sum_{subregions} \hat{I}_i \\ var(\hat{I}) = \hat{\sigma_I}^2 & = & \sum_{subregions} \hat{\sigma_i}^2 \end{array}\right\} \qquad (3)$$

and

$$\left.\begin{array}{rcl} \hat{I}_{AV} & = & \sum_{subregions} \hat{I}_{i,AV} \\ var(\hat{I}_{AV}) = \hat{\sigma}_{I,AV}^2 & = & \sum_{subregions} \hat{\sigma}_{i,AV}^2 \end{array}\right\} \qquad (4)$$

where $\hat{\sigma}_{i,AV}^2$ is the variance of $\hat{I}_{i,AV}$.

Both the usual estimator Eq.(1) and the new estimator Eq.(2) are introduced in the routine DICE version 1.3 and either use of the former or the latter can be selected with setting either `FALSE` or `TRUE` to the boolean constant `ANTITH`.

3 Results

We estimate several definite integrals given in Ref.[5] for test of the new estimator Eq.(2). They are refered as J_i, $i = 1, 2, 3, 4, 5$ in the last paper[9] whose expressions are as follows:

$$J_1 = \int_V e^{-x_1^2 - x_2^2 - x_3^2 - x_4^2} dV, \qquad (5)$$

where V is the region $x_i \geq 0$ and $\sum x_i^2 \leq 1$,

$$J_2 = \int_{-1}^{1}\int_{-1}^{1} |x^2 + y^2 - 0.25| dxdy, \qquad (6)$$

$$J_3 = \int_{0}^{1}\int_{0}^{1} \frac{1}{1 - xy} dxdy, \qquad (7)$$

$$J_4 = \int_{0}^{1}\int_{0}^{1} |x - y|^{1/2} dxdy \qquad (8)$$

and

$$J_5 = \int_{0}^{1}\int_{0}^{1}\int_{0}^{1} \frac{dxdydz}{3 - \cos \pi x - \cos \pi y - \cos \pi z} . \qquad (9)$$

Both values of Eq.(3) and Eq.(4) are computed with two cases of input error, ERRIN $=10^{-4}$ and 10^{-5}. Ten different values of the input parameter for random sampling NSAMPL $= 10, 20, 30, 40, 50, 60, 70, 80, 90$ and 100 are used to see dependence on number of sampling points in each subregion in all computations for figures 1,3,4,5 and 6.

Fig. 1 shows results of the integral J_1. The output list, one of ten outputs of J14AV jobs, with input parameters NSAMPL $= 100$ and ERRIN $= 10^{-4}$, is shown in Fig. 2. The notations J14 and J14AV express the results of the integral J_1 with input error 10^{-4} and AV means use of the new estimator with antithetic variates. J15 and J15AV express the results of the integral J_1 with input error 10^{-5}.

The results of integrals J_2, J_3, J_4 and J_5 with input errors ERRIN $= 10^{-4}$ and 10^{-5} are shown in figures 3, 4, 5 and 6. The same notation as Fig. 1 to express the prerequisites for computation, subscript number of J_2, input error 10^{-4} or 10^{-5} and no AV or AV such that J24, J25, J24AV, J25AV and so on are used to distinguish plot symbols and colors in each figures. The Lmax values depicted are the deepest level of division to obtain each estimate. The deepest level of division means the maximum values of Lmax in the output of execution of the routine DICE v1.3.

True values of the definite integrals J_1, J_2, J_3, J_4 and J_5 are shown by a solid line in each figure. The left axes of figures 1, 3, 4, 5 and 6 are linear scale and the value of scale is used for the integral estimates. The right axes of figures 1, 3, 4, 5 is linear scale but that of figure 6 is log scale. The values of right axes are used for the number of integrand calls required to obtain a result of integration.

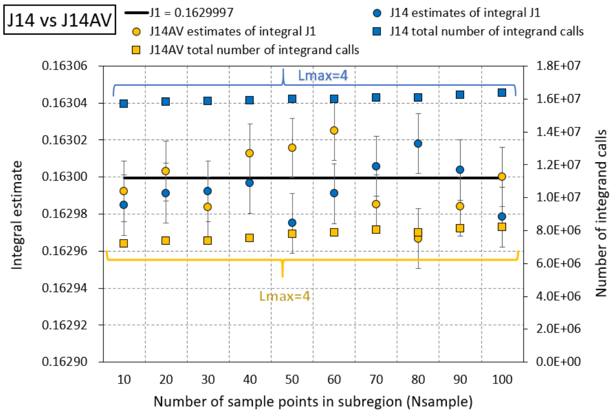
4 Discussions

The integral J_1 is a good example of definite integral of which integrand is smooth function to test the new estimator. In Fig.1(a) all estimates of the integral J_1 are correctly distributed around the true value of the integral within 3 standard deviations. The total numbers of function calls to estimate the integral value by using the new estimator is about half of the usual estimator with same input error 10^{-4}. It means that the new estimator has cut the variance in half.

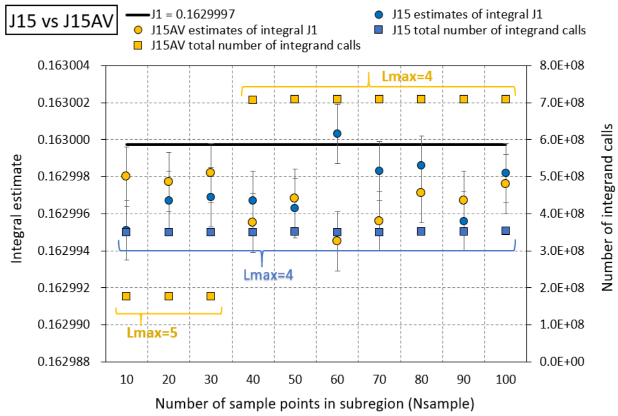
In Fig.1(b) the input error is one order of magnitude smaller than that of Fig.1(a). The central values of the estimates are smaller than the true value except for the estimate of NSAMPL $= 60$ with using Eq.(3). Most of the results are in the correct range, however, some of them are a bit smaller than the true value even if 3 standard deviations are taken into account. The numbers of function calls to calculate the new estimates of the integral with using Eq.(4) are about half of the numbers with using Eq.(3) for three cases of the input parameter NSAMPL $=$ 10, 20 and 30. However for other 7 values of the parameter NSAMPL $=$ 40, 50, 60, 70, 80, 90 and 100, the former is two times as large as the latter. This means that small values of NSAMPL are recommended for variance reduction when using the new estimator. One should note that smaller values of NSAMPL result in deeper level of division, as evidenced by the value of Lmax, resulting in higher efficiency.

The calculation of the integral value by DICE is iteratively repeated. Fig.2 shows the output of J14AV job with the input parameter NSAMPL $= 100$. One can see how the estimates and errors are iteratively calculated and output with cumulative values.

Fig.3 shows the estimates of the definite integral J_2 of which integrand has singularity along the circle $x^2 + y^2 = \left(\frac{1}{2}\right)^2$. The estimates of the integral value are good for almost all input values for NSAMPL in both (a) and (b). The singularity is not a serious matter of integration with DICE. Total number of function calls required to estimate the integral value by using the new estimator is almost one order of magnitude



(a) Comparison of J14 and J14AV (`ERRIN = 0.01%`)

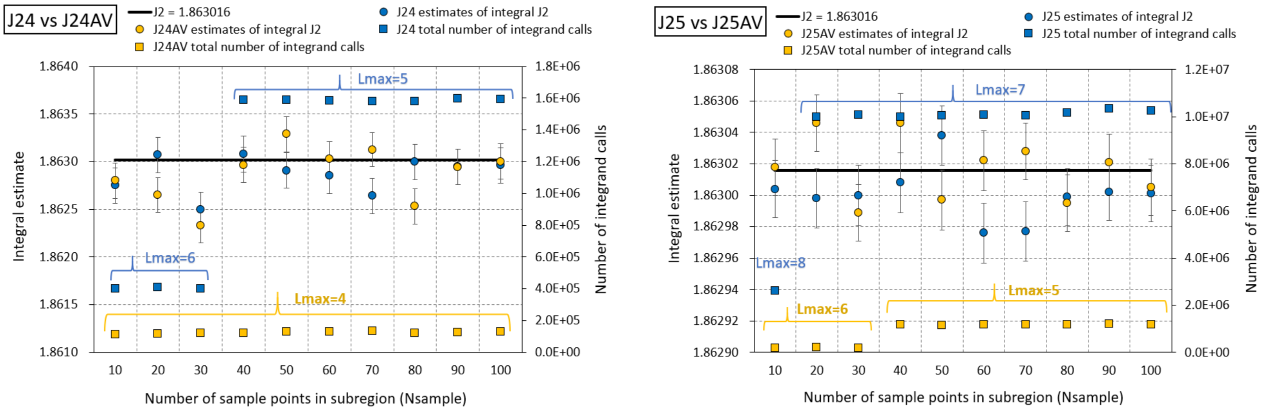


(b) Comparison of J15 and J15AV (`ERRIN = 0.001%`)

Figure 1: 40 estimates of DICE for $J_1 = \int_V e^{-x_1^2-x_2^2-x_3^2-x_4^2} dV$, where V is the region $x_i \geq 0$ and $\sum x_i^2 \leq 1$, are shown by colored circles, (a) 20 estimates of J14 and J14AV with input error `ERRIN =` 10^{-4} and (b) 20 estimates of J15 and J15AV with `ERRIN =` 10^{-5}. The first number 1 expresses the subscript of J_1 and the second numbers 4 and 5 express the negative exponent of the input error `ERRIN`. The true value of J_1 is shown by solid line. In the figures (a) 10 estimates of J14 and (b) 10 estimates of J15, both of which use $\hat{I}$ and $\hat{\sigma_I}$ in Eq.(3), are shown by blue circles and error bars and also (a) 10 estimates of J14AV and (b) 10 estimates of J15AV, both of which use $\hat{I}_{AV}$ and $\hat{\sigma}_{I,AV}$ in Eq.(4) are shown by yellow circles and error bars with respect to different numbers of sample points in subregion, `NSAMPL =` $10, 20, 30, 40, 50, 60, 70, 80, 90$ and 100. Blue square and yellow square show the total number of calls to estimate the integrand function in order to obtain an estimate of integral by using Eq.(3) and Eq.(4), respectively. The `Lmax` values depicted are the deepest level of division to obtain each estimate. They are the maximum values of `Lmax` in each output of executions. Fig.2 shows one of outputs for the J14AV jobs.

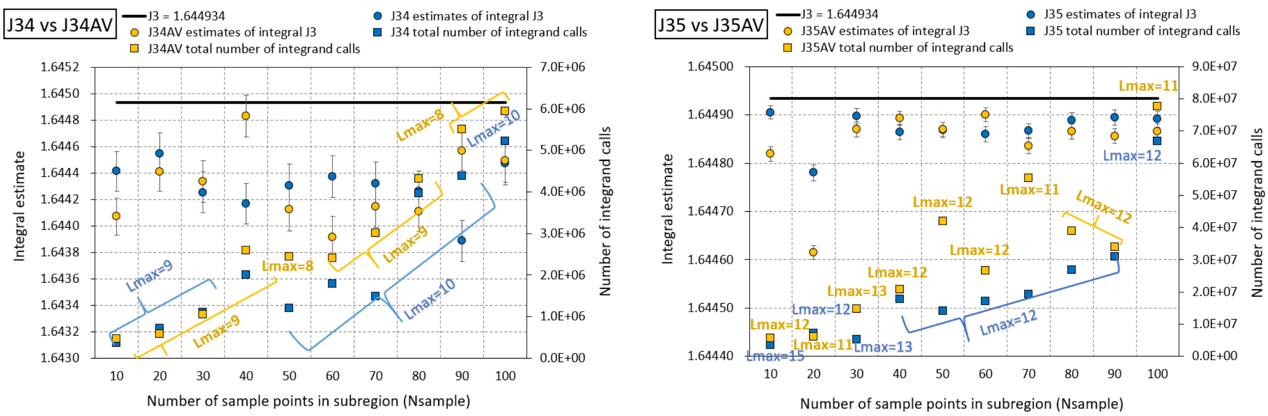
```
auto.f  ( J1 ),  NDIM = 4,  ANTITH = T, HSTSCT = F
                        ***********************************************
                        *                                             *
                        *     JFLAG =    0      CPUMIN = 50000.0min.  *
                        *    NODEMX =  512        NDIM =        4     *
                        *     ITMAX = 1000       ERRIN =   0.01000 %  *
                        *    NSAMPL =  100       JGRID =        0     *
                        *                                             *
                        *   XL( 1) =    0.00E+00  XU( 1) =   1.00E+00 *
                        *   XL( 2) =    0.00E+00  XU( 2) =   1.00E+00 *
                        *   XL( 3) =    0.00E+00  XU( 3) =   1.00E+00 *
                        *   XL( 4) =    0.00E+00  XU( 4) =   1.00E+00 *
                        *                                             *
                        ***********************************************

===============================================================================================
          <  Current  >                  < Cumulative 1 >               < Cumulative 2 >
 IT    Estim._Error          Acc %     Estim._Error          Acc %     Estim._Error          Acc %
===============================================================================================
  0  1.629919_0.000479E-01  0.0294
  1  1.630264_0.000480E-01  0.0294  1.630264_0.000480E-01  0.0294  1.630264_0.000480E-01  0.0294
  2  1.628814_0.000479E-01  0.0294  1.629538_0.000339E-01  0.0208  1.629538_0.000339E-01  0.0208
  3  1.629861_0.000479E-01  0.0294  1.629646_0.000277E-01  0.0170  1.629646_0.000277E-01  0.0170
  4  1.630426_0.000481E-01  0.0295  1.629840_0.000240E-01  0.0147  1.629840_0.000240E-01  0.0147
  5  1.630074_0.000478E-01  0.0294  1.629887_0.000214E-01  0.0132  1.629887_0.000214E-01  0.0132
  6  1.630000_0.000479E-01  0.0294  1.629906_0.000196E-01  0.0120  1.629906_0.000196E-01  0.0120
  7  1.630025_0.000479E-01  0.0294  1.629923_0.000181E-01  0.0111  1.629923_0.000181E-01  0.0111
  8  1.630221_0.000480E-01  0.0294  1.629960_0.000170E-01  0.0104  1.629960_0.000170E-01  0.0104
  9  1.630333_0.000479E-01  0.0294  1.630002_0.000160E-01  0.0098  1.630002_0.000160E-01  0.0098


================================================================================
 IT day/hh:mm:secnd Lmin Lmax Limit    #sampling0     #sampling1     #sampling2
================================================================================
  0   0/ 0: 0: 0.04    4    4    4  74256.000      819200.00      819200.00
  1   0/ 0: 0: 0.07    4    4    4  74256.000      819200.00      819200.00
  2   0/ 0: 0: 0.11    4    4    4  74256.000      819200.00      819200.00
  3   0/ 0: 0: 0.15    4    4    4  74256.000      819200.00      819200.00
  4   0/ 0: 0: 0.19    4    4    4  74256.000      819200.00      819200.00
  5   0/ 0: 0: 0.22    4    4    4  74256.000      819200.00      819200.00
  6   0/ 0: 0: 0.26    4    4    4  74256.000      819200.00      819200.00
  7   0/ 0: 0: 0.30    4    4    4  74256.000      819200.00      819200.00
  8   0/ 0: 0: 0.34    4    4    4  74256.000      819200.00      819200.00
  9   0/ 0: 0: 0.37    4    4    4  74256.000      819200.00      819200.00

                             Total:  742560.00      8192000.0      8192000.0

    ***** Execution completely finished *****
          CTIME =        0.37sec
```

Figure 2: Output of DICE to obtain the estimate of J14AV with input parameters `NSAMPL = 100` and `ERRIN =` 10^{-4}. The calculation is iteratively performed to obtain each output of an estimate of integral and its error (standard deviation) and maximum level of division L_{max} per iteration. They are accumulated and printed out together with cumulative estimates, Cumulative 1 and Cumulative 2, at the end of run. Execution of DICE is fully automatic and it terminates when the accuracy of Cumulative 2 becomes equal to or smaller than `ERRIN`.



(a) Comparison of J24 and J24AV, `ERRIN = 0.01%` (b) Comparison of J25 and J25AV, `ERRIN = 0.001%`

Figure 3: 40 estimates of DICE for $J_2 = \int_{-1}^{1}\int_{-1}^{1}|x^2+y^2-0.25|dxdy$ are shown by colored circles in two figures (a) 20 estimates of J24 and J24AV with `ERRIN = ` 10^{-4} and (b) 20 estimates of J25 and J25AV with `ERRIN = ` 10^{-5}. The first number 2 expresses the subscript of J_2 and the second numbers 4 and 5 express the negative exponent of the input error `ERRIN`. The true value of J_2 is indicated by solid line. J24 and J25 use the expression Eq.(3). J24AV and J25AV use the new expression Eq.(4).



(a) Comparison of J34 and J34AV, `ERRIN = 0.01%` (b) Comparison of J35 and J35AV, `ERRIN = 0.001%`

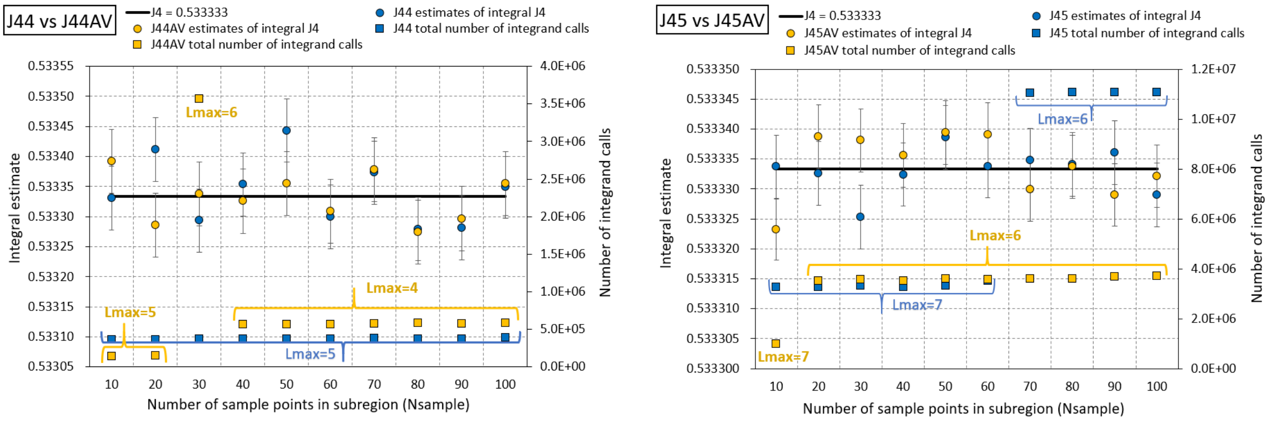
Figure 4: 40 estimates of DICE for $J_3 = \int_0^1\int_0^1 \frac{1}{1-xy}dxdy$ are shown by colored circles in two figures (a) 20 estimates of J34 and J34AV with `ERRIN = ` 10^{-4} and (b) 20 estimates of J35 and J35AV with `ERRIN = ` 10^{-5}. The first number 3 expresses the subscript of J_3 and the second numbers 4 and 5 express the negative exponent of the input error `ERRIN`. The true value of J_3 is indicated by solid line. J34 and J35 use the expression Eq.(3). J34AV and J35AV use the new expression Eq.(4).

smaller than or less than the number required by using the usual estimator for all values of the input parameter `NSAMPL`. This means that the new estimator has reduced the variance by a factor of 10.

The appearance of Fig.4 is different from Fig.1 and Fig.3. With a few exceptions, almost all estimates are less than the true value of J_3, even if their standard deviations are taken into account. The singularity at the point $x = y = 1$ of the integrand of J_3 seems to give the instability of results. The total number of function calls to obtain one estimate of the integral value is not stable. It tends to increase as the number of samples per subregion increases. `Lmax` value is also not stable.

Fig.5 shows that stable and good results of the integral J_4 can be obtained as in Fig.1 and Fig.3. The singularity along the line $x = y$ is not a serious matter of the integration with DICE. However, in this case, the superiority of the new estimator is not yet clear since the numbers of function calls using the new estimator are not always smaller than those using the usual estimator.

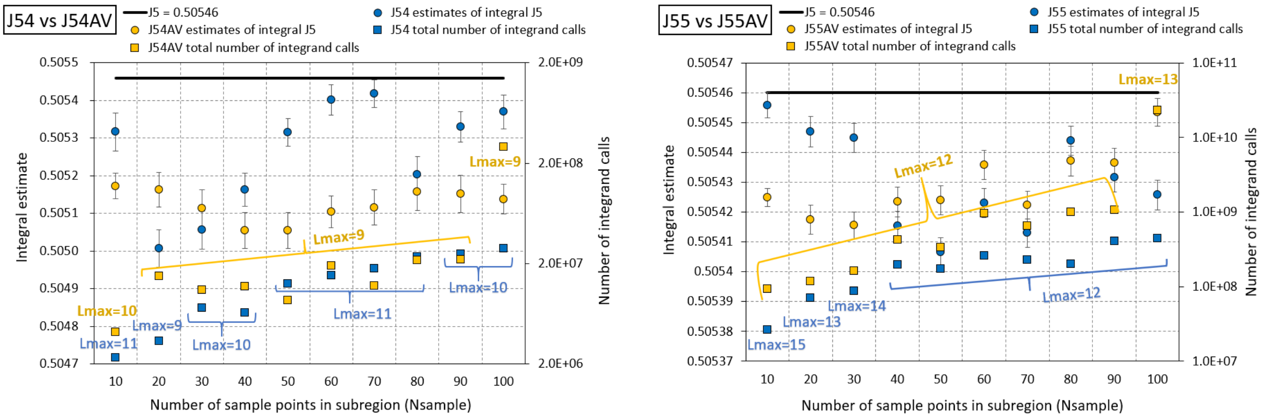
Fig.6 shows the similar aspect as Fig.4. The estimates of DICE for the definite integral J_5 are smaller than true value of the integral. The integrand has singularity at the point $x = y = z = 0$. For the same reason as in Fig.4, the error for the estimate of the integral is not evaluated correctly, resulting in insufficient estimates of the integral J_5.



(a) Comparison of J44 and J44AV, `ERRIN = 0.01%`

(b) Comparison of J45 and J45AV, `ERRIN = 0.001%`

Figure 5: 40 estimates of DICE for $J_4 = \int_0^1 \int_0^1 |x-y|^{1/2} dxdy$ are shown by colored circles in two figures (a) 20 estimates of J44 and J44AV with `ERRIN` = 10^{-4} and (b) 20 estimates of J45 and J45AV with `ERRIN` = 10^{-5}. The first number 4 expresses the subscript of J_4 and the second numbers 4 and 5 express the negative exponent of the input error `ERRIN`. The true value of J_4 is indicated by solid line. J44 and J45 use the expression Eq.(3). J44AV and J45AV use the new expression Eq.(4).



(a) Comparison of J54 and J54AV, `ERRIN = 0.01%`

(b) Comparison of J55 and J55AV, `ERRIN = 0.001%`

Figure 6: 40 estimates of DICE for $J_5 = \int_0^1 \int_0^1 \int_0^1 \frac{dxdydz}{3-\cos\pi x-\cos\pi y-\cos\pi z}$ are shown by colored circles in two figures (a) 20 estimates of J54 and J54AV with `ERRIN` = 10^{-4} and (b) 20 estimates of J55 and J55AV with `ERRIN` = 10^{-5}. The first number 5 expresses the subscript of J_5 and the second numbers 4 and 5 express the negative exponent of the input error `ERRIN`. The true value of J_5 is indicated by solid solid line. J54 and J55 use the expression Eq.(3). J54AV and J55AV use the new expression Eq.(4).

5 Conclusion

We have introduced antithetic variates in automatic integration routine DICE. By using the new estimator we tested several definite integrals given in Ref.[5]. Some of them are smooth integrand function and other have singularity within the integral region. These multiple definite integrals are known as non trivial and good examples for test of the numerical integration.

As the results, the new estimator is found to be effective when the integrand is smooth function and the number of sample points in subregion for random sampling is taken to be small numbers in order to reduce the total number of sample points for the integration.

The present version of DICE does not give correct answer for the definite integral with such a singularity that the integrand becomes infinity at singular point in the integral domain. It can be seen that the estimated values given by DICE version 1.3 for such definite integrals become smaller than the true integral value and the error estimate is also small with using either estimator.

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