Smoothening the Integrands to Increase the Quality of Fluctuationlessness Approximation in Numerical Integration

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Abstract: Recent years brought a new approach which seems to be quite powerful and utilizable with ease in numerical analysis. It is the fluctuationlessness approximation and, univariate or multivariate, an integral can be approximated through its kernel function’s matrix representation by using not it but the image of the matrix representations of the independent variables under that integrand function. Method works well by giving good approximation qualities as long as the integrand behaves sufficiently smooth. Although the method seems to be superior to a lot of existing methods this smoothness related issue stands a problematic agent as in other methods. This work is devoted to the investigation of smoothening possibilities to the integrand.

Key–Words: Integral folding, numerical integration.

1 Introduction

This work is somehow designed to complement the recently developed “Fluctuationlessness Approximation.” This is based on a theorem given and proven by M. Demiralp quite recently. Theorem states that the matrix representation of a univariate function is the image of the matrix representation of the independent variable which is its argument under that function as long as the function is analytic in a domain of the complex plane of the independent variable where the integration is performed. To understand how this theorem is used for the evaluation of the integral of a univariate function. If we define

\[ I \equiv \int_0^1 dxw(x)f(x) \quad (1) \]

where, \( w(x) \) is an appropriate weight function whose integral is 1 for simplicity and consider the Hilbert space, \( \mathcal{H} \), of the univariate functions square integrable on \([0,1]\) then try to relate this integral to the matrix representation of \( f(x) \). If we denote the orthonormal basis functions of \( \mathcal{H} \) by \( u_1(x), ..., u_n(x), ... \) then we can focus on \( \mathcal{H}_n \) which is an \( N \)-dimensional subspace of \( \mathcal{H} \) spanned by \( u_1(x), ..., u_n(x) \) then the matrix representation of \( f(x) \) for this subspace can be denoted by \( M_f^{(n)} \), and satisfy the following equation at the no fluctuation limit.

\[ M_f^{(n)} = f \left( X^{(n)} \right) \quad (2) \]

where, \( e_i^{(n)} \) being \( i \)-th standard unit vector whose only nonzero element is 1 and located at the \( i \)-th position of the vector,

\[ e_i^T M_f^{(n)} e_j = \int_0^1 dxw(x)u_i(x)f(x)u_j(x) \]
\[ e_i^T X^{(n)} e_j = \int_0^1 dxw(x)u_i(x)xu_j(x) \quad (3) \]

Hence, \( X^{(n)} \) is the matrix representation of the independent variable \( x \) for \( \mathcal{H}_n \).

\( u_i \) basis functions can be constructed from the functions set 1, \( x, ..., x^n, ... \) via an appropriate orthonormalization procedure by taking this terms into the procedure in ascending powers. This orthonormalization will apparently leave \( u_1 \) as the constant function whose value is 1 everywhere in the interval. This brings the following new form of the original integral through a tricky idea.

\[ I \equiv \int_0^1 dxw(x)u_1(x)f(x)u_1(x) \]
\[ \equiv e_1^{(n)^T} M_f^{(n)} e_1^{(n)} = e_1^{(n)^T} f \left( X^{(n)} \right) e_1^{(n)} \quad (4) \]

The matrix \( X^{(n)} \) is symmetric therefore it has a spectrum on the real axis. Beyond this, it must be confined into the interval \([0,1]\) since it is the matrix representation of \( x \) over the basis set orthogonal over that interval. All eigenvalues are discrete. If we denote the...
\(i\)-th eigenvalue and corresponding eigenvector by \(\xi_i\)
and \(\mathbf{x}_i\) respectively then we can write the following
spectral resolutions.
\[
\mathbf{X}^{(n)} = \sum_{i=1}^{n} \xi_i \mathbf{x}_i \mathbf{x}_i^T
\]  
(5)
\[
f \left( \mathbf{X}^{(n)} \right) = \sum_{i=1}^{n} f \left( \xi_i \right) \mathbf{x}_i \mathbf{x}_i^T
\]  
(6)
which imply
\[
\mathcal{I} = \sum_{i=1}^{n} f \left( \xi_i \right) \left( \mathbf{e}_i^{(n)} \right) (\mathbf{x}_i)^2
\]  
(7)
This confirms what we have said before. That is, the
integral value is composed of the kernel function’s values at the eigenvalues of universal independent variable matrix representation within the no fluctuation limit.

(7) is a quadrature formula in fact, however, its construction philosophy is different than the existing ones. This formula produces approximation values whose qualities compete with the standing methods and this quality increases quite rapidly as \(n\) grows.

Since it is better to work with rather less dimensions to stay far from the complexities and expenses coming from high dimensionality we may need to develop certain tools accelerating the convergence of the method above. One way to do so is the smoothening of the integrand of the integral by appropriate transformations because higher curvatures in the kernels result in steep growths and therefore great error accumulations. This work focuses on this opportunity.

Paper is organised as follows. The second section covers an illustrative example. The third section gives the conceptual background of the smoothening procedure which can also be called Integral Folding. The third section covers an illustrative example. The fourth section is for the conclusion.

2 Integrand Smoothening
It is possible to uniquely separate any \(g(x)\) function analytic on \([0,1]\) into odd and even functions. This permits us to write
\[
g \left( \frac{1+x}{2} \right) = \frac{1}{2} \left[ g \left( \frac{1+x}{2} \right) + g \left( \frac{1-x}{2} \right) \right] + \frac{1}{2} \left[ g \left( \frac{1+x}{2} \right) - g \left( \frac{1-x}{2} \right) \right]
\]  
(8)
Here the first large bracketed term is an even function since it remains same when all appearances of \(x\) are replaced by \(-x\) whereas the second term is an odd function and reverses its sign under the same transformation. The weight functions in the integrals we focus here must have no singularities everywhere in \([a, b]\), except the endpoints points where they may have singularities that have differentiable structures. We consider \(f(x)\) as an analytic function in the whole interval including the boundary points.

Consider the integral
\[
I_0 = \int_{0}^{1} dx w_0(x) f_0(x)\]  
(9)
with the weight function \(w_0\) satisfying
\[
\int_{0}^{1} dx w_0(x) = 1
\]  
(10)
Let us transform (9) to another integral not between 0 and 1 but \(-1\) and 1 through the following equalities
\[
y \equiv 2x - 1
\]  
(11)
\[
x \equiv \frac{1+y}{2}
\]  
(12)
and get
\[
I_0 = \frac{1}{2} \int_{-1}^{1} dy w_0 \left( \frac{1+y}{2} \right) f_0 \left( \frac{1+y}{2} \right)
\]  
(13)
Separating \(w_0(\frac{1+y}{2})\) and \(f_0(\frac{1+y}{2})\) into odd-even functions, we have \(I_0\) in the form of sum of two even functions because the odd terms are equal to zero on the interval \([-1, 1]\) and get
\[
I_0 = \frac{1}{4} \int_{0}^{1} dy \left[ w_0 \left( \frac{1+y}{2} \right) + w_0 \left( \frac{1-y}{2} \right) \right]
\]  
\[
\left[ f_0 \left( \frac{1+y}{2} \right) + f_0 \left( \frac{1-y}{2} \right) \right]
\]  
\[
+ \frac{1}{4} \int_{0}^{1} dy \left[ w_0 \left( \frac{1+y}{2} \right) - w_0 \left( \frac{1-y}{2} \right) \right]
\]  
\[
\left[ f_0 \left( \frac{1+y}{2} \right) - f_0 \left( \frac{1-y}{2} \right) \right]
\]  
(14)
It is convenient to study this equation in two parts. As we see here, \(I_0\) is the sum of two integrals which
can be denoted by $I_1$ and $I_2$ respectively. Using $\sqrt{y}$ instead of $y$ in $I_1$, we have

$$I_1 = \frac{1}{8} \int_0^1 \frac{dy}{\sqrt{y}} \left[ w_0 \left( \frac{1 + \sqrt{y}}{2} \right) + w_0 \left( \frac{1 - \sqrt{y}}{2} \right) \right]$$

$$\times \left[ f_0 \left( \frac{1 + \sqrt{y}}{2} \right) + f_0 \left( \frac{1 - \sqrt{y}}{2} \right) \right]$$

(15)

Unless having $f_0(\frac{1}{2})$ or $w_0(\frac{1}{2})$ equal to zero, we have a singularity at the point where $y = 0$. To overcome this difficulty, we add and subtract a term providing the second bracketed term, which consists of terms of $f(x)$ function, goes to zero fast by $\sqrt{y}$ going to zero.

$$I_1 = \frac{1}{8} \int_0^1 \frac{dy}{\sqrt{y}} \left[ w_0 \left( \frac{1 + \sqrt{y}}{2} \right) + w_0 \left( \frac{1 - \sqrt{y}}{2} \right) \right]$$

$$\times \left[ f_0 \left( \frac{1 + \sqrt{y}}{2} \right) + f_0 \left( \frac{1 - \sqrt{y}}{2} \right) - 2f_0 \left( \frac{1}{2} \right) \right]$$

$$+ \frac{f_0 \left( \frac{1}{2} \right)}{4} \int_0^1 \frac{dy}{\sqrt{y}} \left[ w_0 \left( \frac{1 + \sqrt{y}}{2} \right) + w_0 \left( \frac{1 - \sqrt{y}}{2} \right) \right]$$

(16)

In this formula the first factor $1/\sqrt{y}$ can be considered as a part of in the second bracketed factor of the first integral. This adds a branch point type integrable singularity around zero to that expression. The new form of the term still goes to zero when $y$ diminishes to zero from the positive values. The branch cut can be taken between minus infinity and zero permitting us to have a convergent integral.

The abovementioned move of $\sqrt{y}$ removes the singularity at $y = 0$ from the weight function. However, it leaves (10) invalid now. One other point is that, after integral folding, the original function may no longer be analytic on the end points. Hence we need to relax the continuity impositions on it at these points. Therefore it is better to write

$$\sigma_1 \equiv \frac{1}{0} \int dx \left[ w_0 \left( \frac{1 + x}{2} \right) + w_0 \left( \frac{1 - x}{2} \right) \right]$$

(17)

$$w_1(x) \equiv \frac{1}{\sigma_1} \left[ w_0 \left( \frac{1 + x}{2} \right) + w_0 \left( \frac{1 + x}{2} \right) \right]$$

(18)

$$f_1(x) \equiv \frac{\sigma_1}{8 \sqrt{x}} \left[ f_0 \left( \frac{1 + x}{2} \right) + f_0 \left( \frac{1 - x}{2} \right) \right. \right.$$

$$\left. - 2f_0 \left( \frac{1}{2} \right) \right]$$

(19)

And finally we reach to the structure below

$$I_1 = \frac{1}{0} \int dx w_1(x) f_1(x) + f_0 \left( \frac{1}{2} \right)$$

(20)

that is similar to (9) for $I_1$. Now we should do a similar analysis for $I_2$, the second integral in (16). Expanding the integral interval into $[-1, 1]$ we get

$$I_2 = \frac{1}{4} \int_0^1 dy \frac{\sqrt{y}}{w_0(\sqrt{y})} \left[ f_0(\sqrt{y}) - f_0 \left( \frac{1}{2} \right) \right]$$

(21)

where the replacement of $y$ by $(2\sqrt{y} - 1)$ leads us to the following structure

$$I_2 = \frac{1}{4} \int_0^1 dy \frac{\sqrt{y}}{w_0(\sqrt{y})} \left[ f_0(\sqrt{y}) - f_0 \left( \frac{1}{2} \right) \right]$$

(22)

where the bracketed term can be set equal to zero at the point $\sqrt{y} = 0$ by adding and subtracting constant terms without changing the whole equation

$$I_2 = \frac{1}{4} \int_0^1 dy \frac{\sqrt{y}}{w_0(\sqrt{y})}$$

$$\times \left[ f_0(\sqrt{y}) - f_0 \left( \frac{1}{2} \right) \right]$$

$$+ \frac{1}{4} \left[ f_0(0) - f_0(1) \right] \int_0^1 dy \frac{\sqrt{y}}{w_0(\sqrt{y})}$$

(23)

Considering the fact that the term

$$\int_0^1 dy \frac{\sqrt{y}}{w_0(\sqrt{y})} = \int_0^1 dy w_0(y)$$

(24)

is equal to 1, we simplify the equation. Using the definitions

$$\sigma_2 \equiv \int_0^1 dx w_0(\sqrt{x})$$

(25)

$$w_2(x) \equiv \frac{1}{\sigma_2} w_0(\sqrt{x})$$

(26)

$$f_2(x) \equiv \frac{\sigma_2}{4 \sqrt{x}} \left[ f_0(\sqrt{y}) - f_0 \left( \frac{1}{2} \right) \right. \right.$$

$$\left. - f_0(0) + f_0(1) \right]$$

(27)
the following structure is obtained for $I_2$

$$I_2 = \int_0^1 dx w_2(x) f_2(x) + \frac{1}{2} [f_0(0) - f_0(1)]$$

Finally what we have done up to here is the conversion of (9) to the form of $I_1 + I_2$ as given below

$$I_0 = \int_0^1 dx w_0(x) f_0(x)$$

$$= \int_0^1 dx w_1(x) f_1(x) + \int_0^1 dx w_2(x) f_2(x)$$

$$+ \frac{1}{2} [f_0(0) - f_0(1)]$$

We call the steps up to this result “Scaled Interval Folding” since the transformation first extends the interval to a larger one and then folds its one part onto other and during this action a coordinate transformation somehow rescales the integration variable. However, this procedure in fact is nothing else but just the smoothingenless theorem here since the weight function has the form of approximation in our illustrative implementations here. We do not attempt to apply the fluctuationlessness approximation here since our basic purpose is to investigate the positive contributions of integrand smoothening to the numerical convergence.

3 An Illustrative Example

For a deeper understanding, we can study on a simple integral whose value has an analytical expression. Consider the integral

$$\int_0^1 dx e^{\alpha x}$$

where the parameter $\alpha$ plays the role of controlling the smoothness. Greater its values less smoothness in the integrand.

Here $f_0$ and $w_0$ are taken as

$$w_0(x) \equiv 1, \quad f_0(x) \equiv e^{\alpha x}$$

Applying mean value estimated scaled interval folding, that is, taking $x_1$ and $x_2$ equal to $1/2$, we get the result given below since the weight function has the value $1$

$$I \approx \frac{\sqrt{2}}{4} \left[ e^{\alpha \frac{\sqrt{2} + 1}{2 \sqrt{2}}} + e^{\alpha \frac{\sqrt{2} - 1}{2 \sqrt{2}}} - 2 e^{\frac{\alpha}{2}} \right]$$

$$+ \frac{\sqrt{2}}{4} \left[ e^{\frac{\sqrt{2}}{2}} - e^{\alpha \frac{\sqrt{2} - 1}{2 \sqrt{2}}} - 1 + e^{\alpha} \right]$$

This approximation is used for different $\alpha$ values and the results are given in Table 1. As seen from Table 1, the relative error gets higher for bigger absolute $\alpha$ values. This is because we use a constant function everywhere in the interval as the approximation of the integrand. As long as the integrand is sufficiently smooth.
Table 1: Results for \( \int_{0}^{1} dx e^{\alpha x} \)

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>Exact</th>
<th>Approx.</th>
<th>Rel. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2.0</td>
<td>0.4323323</td>
<td>0.4514373</td>
<td>-0.0441905</td>
</tr>
<tr>
<td>-1.0</td>
<td>0.6321205</td>
<td>0.6367273</td>
<td>-0.0072878</td>
</tr>
<tr>
<td>-0.5</td>
<td>0.7869386</td>
<td>0.7879218</td>
<td>-0.0012492</td>
</tr>
<tr>
<td>0.5</td>
<td>1.2974425</td>
<td>1.2974346</td>
<td>-0.0000060</td>
</tr>
<tr>
<td>1.0</td>
<td>1.7182818</td>
<td>1.7138902</td>
<td>0.0025558</td>
</tr>
<tr>
<td>2.0</td>
<td>3.1945280</td>
<td>3.1026430</td>
<td>0.0287632</td>
</tr>
<tr>
<td>5.0</td>
<td>29.4826318</td>
<td>18.5480109</td>
<td>0.3708834</td>
</tr>
</tbody>
</table>

the error will be low. Since greater absolute \( \alpha \) values increases the smoothness the relative error in integral value will obviously increases. This error can be decreased by using sufficiently narrow subintervals instead of just the whole interval of the integration. The other alternative is to combine this method with the fluctuationlessness approximation, in other words, by using more than one quadrature points.

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4 Conclusion

The approach introduced in this paper is a basic method that can be combined with any numerical integration method to increase the approximation quality. Actually this new method was developed as an answer to the question “How can we get better approximation using Fluctuationless Expansion Method [1]?"and the main idea was to supress the fluctuations in the function behavior by decreasing its curvature. It is possible to construct different versions of the scaled interval folding methods by using different coordinate transformations. Their recursive utilization may heal also a lot of undesired results. These are now under intense study.

References:


