Numerical Techniques for the Evaluation of Multi-Dimensional Integral Equations

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1. Numerical Derivation of the trapezoidal rule for the 2-D case with constant integration limits

In Section 4.6 of “Numerical Recipes in Fortran 77”, second edition, you can find a brief discussion of when to use different types of numerical methods for evaluating multidimensional integrals.

For the purposes of this course, I am going to show you how to extend the one-dimensional integral evaluation to n-dimensional integral evaluation. This techniques relies upon you have rather simple boundaries to the integral.

For integrals in one dimension, we could start with something simple like the trapezoidal rule.

$$\int_{a}^{b} f(x)dx \approx \frac{h}{2} \left[ f(a) + f(b) + 2\sum_{i=2}^{n_x} f(x_i) \right]$$ (1.1)

Now if we have a 2-D integral we write this as:

$$I_{2D} = \int_{x_0}^{x_f} \int_{y_0}^{y_f} f(x,y)dydx = \int_{x_0}^{x_f} g(x)dx$$ (1.2)

where

$$g(x) = \int_{y_0}^{y_f} f(x,y)dy \approx \frac{h_y}{2} \left[ f(x,y_0) + f(x,y_f) + 2\sum_{j=2}^{n_y} f(x,y_j) \right]$$ (1.3)

Substituting the discretized approximation for g(x) in equation (1.3) into equation (1.2) we have

$$\int_{x_0}^{x_f} \int_{y_0}^{y_f} f(x,y)dydx \approx \frac{h_y}{2} \int_{x_0}^{x_f} \left[ f(x,y_0) + f(x,y_f) + 2\sum_{j=2}^{n_y} f(x,y_j) \right]dx$$ (1.4)

Well, we can repeat the application of the trapezoidal rule:

$$I_{2D} \approx \frac{h_y}{2} \left[ \frac{h_x}{2} \left[ f(x_0,y_0) + f(x_0,y_f) + 2\sum_{i=2}^{n_x} f(x_0,y_i) \right] \right]$$

$$+ \frac{h_y}{2} \left[ \frac{h_x}{2} \left[ f(x_f,y_0) + f(x_f,y_f) + 2\sum_{i=2}^{n_x} f(x_f,y_i) \right] \right]$$

$$+ 2\sum_{j=2}^{n_y} \frac{h_y}{2} \left[ f(x_0,y_j) + f(x_f,y_j) + 2\sum_{i=2}^{n_x} f(x_i,y_j) \right]$$ (1.5)

Now we can simplify this as much as possible,
If we add up the number of function evaluations, we can see that we have $n_x n_y$ function evaluations. If $n_x = n_y = n$, then we have $n^2$ function evaluations for a 2-D integral. If we need to evaluate an $m$-dimensional integral, then we will have $n^m$ function evaluations.
2. Numerical Derivation of the trapezoidal rule for the 3-D case with constant integration limits

Now if we have a 3-D integral we write this as:

\[ I_{3D} = \int_{x_0}^{x_f} \int_{y_0}^{y_f} \int_{z_0}^{z_f} f(x, y, z) \, dz \, dy \, dx = \int_{x_0}^{x_f} h(x) \, dx \]  
(2.1)

where

\[ h(x) = \int_{y_0}^{y_f} \int_{z_0}^{z_f} f(x, y, z) \, dz \, dy = \int_{y_0}^{y_f} g(x, y) \, dy \]  
(2.2)

where

\[ g(x, y) = \int_{z_0}^{z_f} f(x, y, z) \, dz \]  
(2.3)

Using the trapezoidal rule approximation:

\[ g(x, y) = \int_{z_0}^{z_f} f(x, y, z) \, dz \approx \frac{h_z}{2} \left[ f(x, y, z_0) + f(x, y, z_f) + 2 \sum_{i=2}^{n_z} f(x, y, z_i) \right] \]  
(2.4)

Substituting the discretized approximation for \( g(x, y) \) from equation (2.4) into equation (2.2) we have

\[ h(x) = \int_{y_0}^{y_f} \int_{z_0}^{z_f} f(x, y, z) \, dz \, dy = \int_{y_0}^{y_f} \frac{h_z}{2} \left[ f(x, y, z_0) + f(x, y, z_f) + 2 \sum_{i=2}^{n_z} f(x, y, z_i) \right] dy \]  
(2.5)

Well, we can repeat the application of the trapezoidal rule:

\[ h(x) = \frac{h_y}{2} \left[ f(x, y_0, z_0) + f(x, y_0, z_f) + 2 \sum_{i=2}^{n_y} f(x, y_0, z_i) \right] + \frac{h_z}{2} \left[ f(x, y_f, z_0) + f(x, y_f, z_f) + 2 \sum_{i=2}^{n_z} f(x, y_f, z_i) \right] + 2 \frac{h_z}{2} \sum_{i=2}^{n_z} \left[ f(x, y_0, z_i) + f(x, y_f, z_i) + 2 \sum_{j=2}^{n_y} f(x, y_j, z_i) \right] \]  
(2.6)

Now we can simplify this as much as possible,

\[ h(x) \approx \frac{h_y h_z}{4} \left[ f(x, y_0, z_0) + f(x, y_0, z_f) + f(x, y_f, z_0) + f(x, y_f, z_f) + 4 \sum_{j=2}^{n_y} \sum_{i=2}^{n_z} f(x, y_j, z_i) + 2 \sum_{i=2}^{n_z} \left[ f(x, y_0, z_i) + f(x, y_f, z_i) \right] + 2 \sum_{j=2}^{n_y} \left[ f(x, y_j, z_0) + f(x, y_j, z_f) \right] \right] \]  
(2.7)
Now we can apply the trapezoidal rule one more time:

\[
I_{3D} = \frac{h_x h_y h_z}{2^3} \left[ \left\{ f(x_0, y_0, z_0) + f(x_0, y_0, z_1) + f(x_0, y_1, z_0) + f(x_0, y_1, z_1) + \frac{1}{2} \sum_{i=2}^{n_x} \left[ f(x_0, y_i, z_0) + f(x_0, y_i, z_1) \right] \right\} + 2 \sum_{j=2}^{n_y} \left[ f(x_j, y_0, z_0) + f(x_j, y_0, z_1) \right] + 2 \sum_{j=2}^{n_y} \left[ f(x_j, y_1, z_0) + f(x_j, y_1, z_1) \right] + 4 \sum_{j=2}^{n_y} \sum_{j=2}^{n_y} f(x_j, y_j, z_0) + f(x_j, y_j, z_1) \right]
\]

which if we really are bored ten minutes to five on a Wednesday evening, we can rearrange as:

\[
I_{3D} = \frac{h_x h_y h_z}{2^3} \left[ \left\{ f(x_0, y_0, z_0) + f(x_0, y_0, z_1) + f(x_0, y_1, z_0) + f(x_0, y_1, z_1) \right\} + \frac{1}{2} \sum_{i=2}^{n_x} \left[ f(x_0, y_i, z_0) + f(x_0, y_i, z_1) \right] + \frac{1}{2} \sum_{j=2}^{n_y} \left[ f(x_j, y_0, z_0) + f(x_j, y_0, z_1) \right] + \frac{1}{2} \sum_{j=2}^{n_y} \left[ f(x_j, y_1, z_0) + f(x_j, y_1, z_1) \right] + 4 \sum_{j=2}^{n_y} \sum_{j=2}^{n_y} f(x_j, y_j, z_0) + f(x_j, y_j, z_1) \right]
\]

This is the explicit form of the trapezoidal rule applied in 3-dimensions, when the limits of integration are constant.
3. Numerical Derivation of the trapezoidal rule for the 2-D case with variable integration limits

Now if we have a 2-D integral with variable limits of integration, we write this as:

\[
I_{\text{2D}} = \int_{x_0}^{x_f} \int_{y_0(x)}^{y_f(\cdot)} f(x, y) \, dy \, dx = \int_{x_0}^{x_f} g(x) \, dx
\]  
(3.1)

where

\[
g(x) = \frac{y_f(x) - y_0(x)}{2} \left[ f(x, y_0(x)) + f(x, y_f(x)) + 2 \sum_{i=2}^{n_y(x)} f(x, y_i(x)) \right]
\]  
(3.2)

The number of y-intervals, \( n_y(x) \), is now a function of x because the size of the y-range of integration is a function of x. Substituting the discretized approximation for \( g(x) \) in equation (3.2) into equation (3.1) we have

\[
\int_{x_0}^{x_f} \int_{y_0(x)}^{y_f(\cdot)} f(x, y) \, dy \, dx = \int_{x_0}^{x_f} \frac{h_y}{2} \left[ f(x, y_0(x)) + f(x, y_f(x)) + 2 \sum_{i=2}^{n_y(x)} f(x, y_i(x)) \right] \, dx
\]  
(3.3)

Well, we can repeat the application of the trapezoidal rule:

\[
I_{\text{2D}} = \frac{h_x}{2} \left[ \frac{h_y}{2} \left[ f(x_0, y_0(x_0)) + f(x_0, y_f(x_0)) + 2 \sum_{i=2}^{n_y(x_0)} f(x_0, y_i(x_0)) \right] + \frac{h_y}{2} \left[ f(x_1, y_0(x_1)) + f(x_1, y_f(x_1)) + 2 \sum_{i=2}^{n_y(x_1)} f(x_1, y_i(x_1)) \right] \right]
\]  
(3.4)

Now we can simplify this as much as possible,

\[
I_{\text{2D}} = \frac{h_x h_y}{4} \left[ f(x_0, y_0(x_0)) + f(x_0, y_f(x_0)) + f(x_1, y_0(x_1)) + f(x_1, y_f(x_1)) + 2 \sum_{i=2}^{n_y(x_0)} f(x_0, y_i(x_0)) + \sum_{i=2}^{n_y(x_1)} f(x_1, y_i(x_1)) \right] + \sum_{j=2}^{n_x(x_0)} \sum_{i=2}^{n_y(x_j)} f(x_j, y_i(x_j))
\]  
(3.5)
Let’s do an example. Let’s integrate \( f(x, y) = cxy \) over the range \( 0 \leq x \leq 1 \) and \( 0 \leq x \leq y \). Let’s do it analytically first:

\[
I_{2D} = \int_{x_0}^{y_f} \int_{y_0}^{x} f(x, y) \, dy \, dx = \int_{x_0}^{1} cxy \, dy \, dx = \int_{0}^{1} \frac{cxy^2}{2} \, dx = \frac{cx^2}{8} \bigg|_{0}^{1} = \frac{c}{8}
\]  

(3.6)

Now let’s do it analytically with \( \Delta x = \Delta y = h = 0.1 \) \( c = 2 \)

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The numerical solution is \( I_{2D} = 0.2405 \) compared to the exact solution, \( I_{2D} = 0.25 \)
4. Numerical Derivation of the Simpson’s 1/3 rule for the 2-D case with constant integration limits

Now if we have a 2-D integral we write this as:

\[
I_{2D} = \int_{x_0}^{x_f} \int_{y_0}^{y_f} f(x, y) \, dy \, dx = \int_{x_0}^{x_f} g(x) \, dx
\]  

(4.1)

where

\[
g(x) = \frac{y_f}{y_0} \left( f(x, y_o) + f(x, y_f) + 4 \sum_{i=2,4,6}^{n_x-1} f(x, y_i) + 2 \sum_{i=3,5,7}^{n_x-2} f(x, y_i) \right)
\]  

(4.2)

Substituting the discretized approximation for \( g(x) \) in equation (4.2) into equation (4.1) we have

\[
I_{2D} = \int_{x_0}^{x_f} \left( f(x, y_o) + f(x, y_f) + 4 \sum_{i=2,4,6}^{n_x-1} f(x, y_i) + 2 \sum_{i=3,5,7}^{n_x-2} f(x, y_i) \right) \, dx
\]  

(4.3)

Well, we can repeat the application of the trapezoidal rule:

\[
I_{2D} = \frac{h_x}{3} \left( f(x_o, y_o) + f(x_o, y_f) + 4 \sum_{i=2,4,6}^{n_x-1} f(x_o, y_i) + 2 \sum_{i=3,5,7}^{n_x-2} f(x_o, y_i) \right)
\]  

\[
+ \frac{h_y}{3} \left( f(x_f, y_o) + f(x_f, y_f) + 4 \sum_{i=2,4,6}^{n_y-1} f(x_f, y_i) + 2 \sum_{i=3,5,7}^{n_y-2} f(x_f, y_i) \right)
\]  

\[
+ 4 \sum_{j=2,4,6}^{n_y-1} \frac{h_y}{3} \left( f(x_j, y_o) + f(x_j, y_f) + 4 \sum_{j=2,4,6}^{n_y-1} f(x_j, y_i) + 2 \sum_{i=3,5,7}^{n_y-2} f(x_j, y_i) \right)
\]  

(4.4)

\[
+ 2 \sum_{j=3,5,7}^{n_y-2} \frac{h_y}{3} \left( f(x_j, y_o) + f(x_j, y_f) + 4 \sum_{j=2,4,6}^{n_y-1} f(x_j, y_i) + 2 \sum_{i=3,5,7}^{n_y-2} f(x_j, y_i) \right)
\]

Now we can simplify this as much as possible,
\[ l_{2D} = \frac{h_x h_y}{9} \left\{ \begin{array}{c} f(x_0, y_0) + f(x_0, y_f) + f(x_f, y_0) + f(x_f, y_f) \\ + 2 \left[ \sum_{i=3,5,7}^{n_x-2} [f(x_0, y_i) + f(x_i, y_0)] + \sum_{j=3,5,7}^{n_y-2} [f(x_j, y_0) + f(x_j, y_f)] \right] \\ + 4 \left[ \sum_{i=2,4,6}^{n_x-1} [f(x_0, y_i) + f(x_i, y_0)] + \sum_{j=2,4,6}^{n_y-1} [f(x_j, y_0) + f(x_j, y_f)] \right] \\ + 8 \left[ \sum_{i=2,4,6}^{n_x-2} \sum_{j=3,5,7}^{n_y-2} f(x_j, y_i) + \sum_{j=3,5,7}^{n_y-2} \sum_{i=2,4,6}^{n_x-2} f(x_j, y_i) \right] \\ + 4 \sum_{j=3,5,7}^{n_y-1} \sum_{i=3,5,7}^{n_x-2} f(x_j, y_i) + 16 \sum_{j=2,4,6}^{n_y-1} \sum_{i=2,4,6}^{n_x-2} f(x_j, y_i) \end{array} \right\} \]