Numerical Techniques for the Evaluation of Multi-Dimensional Integral Equations

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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.

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

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

$$I_{2D} = \int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx = \int_{xo}^{xf} g(x)dx \tag{1.2}$$

where

$$g(x) = \int_{yo}^{yf} f(x,y)dy \approx \frac{h_y}{2}\left[f(x,y_o)+f(x,y_f)+2\sum_{i=2}^{n_y} f(x,y_i)\right] \tag{1.3}$$

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

$$\int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx \approx \int_{xo}^{xf} \frac{h_y}{2}\left[f(x,y_o)+f(x,y_f)+2\sum_{i=2}^{n_y} f(x,y_i)\right]dx \tag{1.4}$$

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

$$I_{2D} \approx \frac{h_x}{2}\left\{\begin{array}{l} \frac{h_y}{2}\left[f(x_o,y_o)+f(x_o,y_f)+2\sum_{i=2}^{n_y} f(x_o,y_i)\right] \\ +\frac{h_y}{2}\left[f(x_f,y_o)+f(x_f,y_f)+2\sum_{i=2}^{n_y} f(x_f,y_i)\right] \\ +2\sum_{j=2}^{n_x}\frac{h_y}{2}\left[f(x_j,y_o)+f(x_j,y_f)+2\sum_{i=2}^{n_y} f(x_j,y_i)\right] \end{array}\right\} \tag{1.5}$$

Now we can simplify this as much as possible,

$$I_{2D} \approx \frac{h_x h_y}{4}\left\{\begin{array}{l} f(x_o,y_o)+f(x_o,y_f)+f(x_f,y_o)+f(x_f,y_f)+4\sum_{i=2}^{n_y}\sum_{j=2}^{n_x} f(x_j,y_i) \\ +2\sum_{i=2}^{n_y}\left[f(x_o,y_i)+f(x_f,y_i)\right]+2\sum_{j=2}^{n_x}\left[f(x_j,y_o)+f(x_j,y_f)\right] \end{array}\right\} \quad (1.6)$$

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:

$$I_{3D} = \int_{xo}^{xf}\int_{yo}^{yf}\int_{zo}^{zf} f(x,y,z)dzdydx = \int_{xo}^{xf} h(x)dx \tag{2.1}$$

where

$$h(x) = \int_{yo}^{yf}\int_{zo}^{zf} f(x,y,z)dzdy = \int_{yo}^{yf} g(x,y)dy \tag{2.2}$$

where

$$g(x,y) = \int_{zo}^{zf} f(x,y,z)dz \tag{2.3}$$

Using the trapezoidal rule approximation:

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

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

$$h(x) = \int_{yo}^{yf}\int_{zo}^{zf} f(x,y,z)dzdy = \int_{yo}^{yf} \frac{h_z}{2}\left[f(x,y,z_o) + f(x,y,z_f) + 2\sum_{i=2}^{n_z} f(x,y,z_i)\right]dy \tag{2.5}$$

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

$$h(x) \approx \frac{h_y}{2}\left\{\begin{array}{l} \frac{h_z}{2}\left[f(x,y_o,z_o) + f(x,y_o,z_f) + 2\sum_{i=2}^{n_z} f(x,y_o,z_i)\right] \\ + \frac{h_z}{2}\left[f(x,y_f,z_o) + f(x,y_f,z_f) + 2\sum_{i=2}^{n_z} f(x,y_f,z_i)\right] \\ + 2\frac{h_z}{2}\sum_{j=2}^{n_y}\left[f(x,y_j,z_o) + f(x,y_j,z_f) + 2\sum_{i=2}^{n_z} f(x,y_j,z_i)\right] \end{array}\right\} \tag{2.6}$$

Now we can simplify this as much as possible,

$$h(x) \approx \frac{h_y h_z}{4}\left\{\begin{array}{l} f(x,y_o,z_o) + f(x,y_o,z_f) + f(x,y_f,z_o) + f(x,y_f,z_f) + 4\sum_{j=2}^{n_y}\sum_{i=2}^{n_z} f(x,y_j,z_i) \\ + 2\sum_{i=2}^{n_z}\left[f(x,y_o,z_i) + f(x,y_f,z_i)\right] + 2\sum_{j=2}^{n_y}\left[f(x,y_j,z_o) + f(x,y_j,z_f)\right] \end{array}\right\} \tag{2.7}$$

Now we can apply the trapezoidal rule one more time:

$$
I_{3D} = \frac{h_x h_y h_z}{2^3}\left[\begin{array}{l}
\left\{\begin{array}{l}
f(x_o,y_o,z_o)+f(x_o,y_o,z_f)+f(x_o,y_f,z_o)+f(x_o,y_f,z_f)+4\sum\limits_{j=2}^{n_y}\sum\limits_{i=2}^{n_z} f(x_o,y_j,z_i) \\
+2\sum\limits_{i=2}^{n_z}\left[f(x_o,y_o,z_i)+f(x_o,y_f,z_i)\right]+2\sum\limits_{j=2}^{n_y}\left[f(x_o,y_j,z_o)+f(x_o,y_j,z_f)\right]
\end{array}\right\} \\
+\left\{\begin{array}{l}
f(x_f,y_o,z_o)+f(x_f,y_o,z_f)+f(x_f,y_f,z_o)+f(x_f,y_f,z_f)+4\sum\limits_{j=2}^{n_y}\sum\limits_{i=2}^{n_z} f(x_f,y_j,z_i) \\
+2\sum\limits_{i=2}^{n_z}\left[f(x_f,y_o,z_i)+f(x_f,y_f,z_i)\right]+2\sum\limits_{j=2}^{n_y}\left[f(x_f,y_j,z_o)+f(x_f,y_j,z_f)\right]
\end{array}\right\} \\
+2\sum\limits_{k=2}^{nx}\left\{\begin{array}{l}
f(x_k,y_o,z_o)+f(x_k,y_o,z_f)+f(x_k,y_f,z_o)+f(x_k,y_f,z_f)+4\sum\limits_{j=2}^{n_y}\sum\limits_{i=2}^{n_z} f(x_k,y_j,z_i) \\
+2\sum\limits_{i=2}^{n_z}\left[f(x_k,y_o,z_i)+f(x_k,y_f,z_i)\right]+2\sum\limits_{j=2}^{n_y}\left[f(x_k,y_j,z_o)+f(x_k,y_j,z_f)\right]
\end{array}\right\}
\end{array}\right] \quad (2.8)
$$

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

$$
I_{3D} = \frac{h_x h_y h_z}{2^3}\left[\begin{array}{l}
\left\{\begin{array}{l}
f(x_o,y_o,z_o)+f(x_o,y_o,z_f)+f(x_o,y_f,z_o)+f(x_o,y_f,z_f) \\
+f(x_f,y_o,z_o)+f(x_f,y_o,z_f)+f(x_f,y_f,z_o)+f(x_f,y_f,z_f)
\end{array}\right\} \\
+2\left\{\begin{array}{l}
\sum\limits_{i=2}^{n_z}\left[f(x_o,y_o,z_i)+f(x_o,y_f,z_i)+f(x_f,y_o,z_i)+f(x_f,y_f,z_i)\right] \\
+\sum\limits_{j=2}^{n_y}\left[f(x_o,y_j,z_o)+f(x_o,y_j,z_f)+f(x_f,y_j,z_o)+f(x_f,y_j,z_f)\right] \\
+\sum\limits_{k=2}^{nx}\left[f(x_k,y_o,z_o)+f(x_k,y_o,z_f)+f(x_k,y_f,z_o)+f(x_k,y_f,z_f)\right]
\end{array}\right\} \\
+4\left\{\begin{array}{l}
\sum\limits_{j=1}^{n_y}\sum\limits_{i=2}^{n_z}\left[f(x_o,y_j,z_i)+f(x_f,y_j,z_i)\right]+\sum\limits_{k=2}^{nx}\sum\limits_{i=2}^{n_z}\left[f(x_k,y_o,z_i)+f(x_k,y_f,z_i)\right] \\
+\sum\limits_{k=2}^{nx}\sum\limits_{j=1}^{n_y}\left[f(x_k,y_j,z_o)+f(x_k,y_j,z_f)\right]
\end{array}\right\} \\
+8\sum\limits_{k=2}^{nx}\sum\limits_{j=1}^{n_y}\sum\limits_{i=2}^{n_z} f(x_k,y_j,z_i)
\end{array}\right] \quad (2.9)
$$

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:

$$I_{2D} = \int_{xo}^{xf} \int_{yo(x)}^{yf(x)} f(x,y)dydx = \int_{xo}^{xf} g(x)dx \tag{3.1}$$

where

$$g(x) = \int_{yo(x)}^{yf(x)} f(x,y)dy \approx \frac{h_y}{2}\left[f(x,y_o(x)) + f(x,y_f(x)) + 2\sum_{i=2}^{n_y(x)} f(x,y_i(x)) \right] \tag{3.2}$$

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

$$\int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx \approx \int_{xo}^{xf} \frac{h_y}{2}\left[f(x,y_o(x)) + f(x,y_f(x)) + 2\sum_{i=2}^{n_y(x)} f(x,y_i(x)) \right]dx \tag{3.3}$$

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

$$I_{2D} \approx \frac{h_x}{2}\left\{ \begin{array}{l} \frac{h_y}{2}\left[f(x_o,y_o(x_o)) + f(x_o,y_f(x_o)) + 2\sum_{i=2}^{n_y(x_o)} f(x_o,y_i(x_o)) \right] \\ + \frac{h_y}{2}\left[f(x_f,y_o(x_f)) + f(x_f,y_f(x_f)) + 2\sum_{i=2}^{n_y(x_f)} f(x_f,y_i(x_f)) \right] \\ + 2\sum_{j=2}^{n_x} \frac{h_y}{2}\left[f(x_j,y_o(x_j)) + f(x_j,y_f(x_j)) + 2\sum_{i=2}^{n_y(x_j)} f(x_j,y_i(x_j)) \right] \end{array} \right\} \tag{3.4}$$

Now we can simplify this as much as possible,

$$I_{2D} \approx \frac{h_x h_y}{4}\left\{ \begin{array}{l} f(x_o,y_o(x_o)) + f(x_o,y_f(x_o)) + f(x_f,y_o(x_f)) + f(x_f,y_f(x_f)) \\ + 2\left[\sum_{i=2}^{n_y(x_o)} f(x_o,y_i(x_o)) + \sum_{i=2}^{n_y(x_f)} f(x_f,y_i(x_f)) + \sum_{j=2}^{n_x} f(x_j,y_o(x_j)) + \sum_{j=2}^{n_x} f(x_j,y_f(x_j)) \right] \\ + 4\sum_{j=2}^{n_x}\sum_{i=2}^{n_y(x_j)} f(x_j,y_i(x_j)) \end{array} \right\} \tag{3.5}$$

Let's do an example. Let's integrate $f(x,y) = cxy$ over the range $0 \le x \le 1$ and $0 \le x \le y$. Let's do it analytically first:

$$I_{2D} = \int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx = \int_0^1\int_0^x cxydydx = \int_0^1 \left[\frac{cxy^2}{2}\right]_0^x dx = \int_0^1 \frac{cx^3}{2}dx = \left.\frac{cx^4}{8}\right|_0^1 = \frac{c}{8} \qquad (3.6)$$

Now let's do it analytically with $\Delta x = \Delta y = h = 0.1$ $c = 2$

i	x	yo(x)	yf(x)	ny(x)	f(x,yo)	f(x,yf)	sum(f(x,yj)	integral(x)
0	0	0	0	0	0	0	0	0
1	0.1	0	0.1	1	0	0.2	0	0.01
2	0.2	0	0.2	2	0	0.4	0.02	0.022
3	0.3	0	0.3	3	0	0.6	0.12	0.042
4	0.4	0	0.4	4	0	0.8	0.36	0.076
5	0.5	0	0.5	5	0	1	0.8	0.13
6	0.6	0	0.6	6	0	1.2	1.5	0.21
7	0.7	0	0.7	7	0	1.4	2.52	0.322
8	0.8	0	0.8	8	0	1.6	3.92	0.472
9	0.9	0	0.9	9	0	1.8	5.76	0.666
10	1	0	1	10	0	2	8.1	0.91
							total	0.2405

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:

$$I_{2D} = \int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx = \int_{xo}^{xf} g(x)dx \tag{4.1}$$

where

$$g(x) = \int_{yo}^{yf} f(x,y)dy \approx \frac{h_y}{3}\left(f(x,y_o) + f(x,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x,y_i) \right) \tag{4.2}$$

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

$$\int_{xo}^{xf}\int_{yo}^{yf} f(x,y)dydx \approx \int_{xo}^{xf} \frac{h_y}{3}\left(f(x,y_o) + f(x,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x,y_i) \right)dx \tag{4.3}$$

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

$$I_{2D} \approx \frac{h_x}{3}\left\{ \begin{array}{l} \frac{h_y}{3}\left(f(x_o,y_o) + f(x_o,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x_o,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x_o,y_i) \right) \\ + \frac{h_y}{3}\left(f(x_f,y_o) + f(x_f,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x_f,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x_f,y_i) \right) \\ + 4\sum_{j=2,4,6}^{n_x-1} \frac{h_y}{3}\left(f(x_j,y_o) + f(x_j,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x_j,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x_j,y_i) \right) \\ + 2\sum_{j=3,5,7}^{n_x-2} \frac{h_y}{3}\left(f(x_j,y_o) + f(x_j,y_f) + 4\sum_{i=2,4,6}^{n_y-1} f(x_j,y_i) + 2\sum_{i=3,5,7}^{n_y-2} f(x_j,y_i) \right) \end{array} \right\} \tag{4.4}$$

Now we can simplify this as much as possible,

$$I_{2D} \approx \frac{h_x h_y}{9}\left\{\begin{bmatrix} f(x_o,y_o)+f(x_o,y_f)+f(x_f,y_o)+f(x_f,y_f) \\ +2\left(\sum_{i=3,5,7}^{n_y-2}\left[f(x_o,y_i)+f(x_f,y_i)\right]+\sum_{j=3,5,7}^{n_x-2}\left[f(x_j,y_o)+f(x_j,y_f)\right]\right) \\ +4\left(\sum_{i=2,4,6}^{n_y-1}\left[f(x_o,y_i)+f(x_f,y_i)\right]+\sum_{j=2,4,6}^{n_x-1}\left[f(x_j,y_o)+f(x_j,y_f)\right]\right) \\ +8\left(\sum_{j=2,4,6}^{n_x-1}\sum_{i=3,5,7}^{n_y-2}f(x_j,y_i)+\sum_{j=3,5,7}^{n_x-2}\sum_{i=2,4,6}^{n_y-1}f(x_j,y_i)\right) \\ +4\sum_{j=3,5,7}^{n_x-2}\sum_{i=3,5,7}^{n_y-2}f(x_j,y_i)+16\sum_{j=2,4,6}^{n_x-1}\sum_{i=2,4,6}^{n_y-1}f(x_j,y_i) \end{bmatrix}\right\} \tag{4.5}$$