The Trapezium and Simpson's rules extended to three dimensions, with an application

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When limnologists (scientists who study lakes) wish to find the volume of a lake they find depth contours, where the depth of the lake is the same at any two points on the given contour. Let $A(x)$ be the area contained in the contour at depth x. The function $A(x)$ is assumed to be strictly decreasing with $A(D) = 0$ where D is the maximum depth of the lake. The standard formula for the volume that they use is

$$V \approx \sum_{k=1}^{n} \frac{A_{k-1} + A_k + \sqrt{A_{k-1}A_k}}{3}\Delta x, \text{ where } A_k = A\left(\frac{kD}{n}\right)$$

over $n + 1$ equally-spaced depth contours with $\Delta x = \frac{D}{n}$. This approach is very well analysed in [1].

In this Article we will take a less sophisticated approach. The fact that $A(x)$ is assumed to be strictly decreasing seems to be a considerable limitation. We might have a lake where the bottom undulates or even with a beautiful island in the middle of it. We will consider that our scientists do not have much technology available. They have a marked line of rope, with a lead weight attached to one end, that they can deploy from a rowing boat, which they can position accurately on a two-dimensional grid of the lake's surface (if they wanted to be a bit more modern they could have a ship with a depth sounder).

A rectangular grid of size $l_1 \times l_2$ is created to just contain, at least, the surface of the lake. The grid lines are equally spaced at width h apart where $l_1 = n_1 h$ and $l_2 = n_2 h$ with $n_1, n_2 \in \mathbb{N}$. The depth of the lake is denoted by $f_{i,j}$ is found at all the points (ih, jh), $0 \leqslant i \leqslant n_1$, $0 \leqslant j \leqslant n_2$. If the grid point is strictly on dry land around the lake or on an island then that particular depth would be taken as 0.

Let the unknown function that represents the depth of the lake be $f(x, y)$.

To emulate the derivation of the trapezium rule we will first approximate this by the function $f_1(x, y) = a + bx + cy + dxy$ which is only linear in either x or y. We will consider the volume generated by this function on one grid square with coordinates given by (0, 0), (0, h), (h, 0), (h, h). This one grid square is representative of any other grid square but keeps the algebra simpler. The volume given by this function on this grid square will be

$$V_T = \int_0^h \int_0^h (a + bx + cy + dxy)\,dx\,dy = \int_0^h ah + \frac{bh^2}{2} + cyh + \frac{dyh^2}{2}dy$$

$$= ah^2 + \frac{bh^3}{2} + \frac{ch^3}{2} + \frac{dh^4}{4} = \frac{h^2}{4}(4a + 2bh + 2ch + dh^2). \qquad (1)$$

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Now $f_{0,0} = a$, $f_{0,1} = a + ch$, $f_{1,0} = a + bh$, $f_{1,1} = a + bh + ch + dh^2$ so eliminating a, b, c, d from (1) we have

$$V_T = \frac{h^2}{4}\left(f_{0,0} + f_{0,1} + f_{1,0} + f_{1,1}\right).$$

This result has the expected symmetry and fits with a dimensions check. The same result can be similarly achieved for any of the other grid squares. So an approximation for V will be

$$\frac{h^2}{4}\left(\text{a linear combination of the depths at the grid points}\right).$$

The four corner points of the grid will have a coefficient of 1, the edge points of the grid that are not corner points will have a coefficient of 2 and all the interior points of the grid will have a coefficient of 4. This approximation could be expressed as

$$V \approx \frac{h^2}{4} \times$$

$$\left\{1 \times \left(f_{0,0} + f_{0,n_2} + f_{n_1,0} + f_{n_1,n_2}\right) + 2 \times \left(\sum_{j=1}^{n_2-1} f_{0,j} + \sum_{j=1}^{n_2-1} f_{n_1,j} + \sum_{i=1}^{n_1-1} f_{i,0} + \sum_{i=1}^{n_1-1} f_{i,n_2}\right) + 4 \times \left(\sum_{i=1}^{n_1-1}\sum_{j=1}^{n_2-1} f_{i,j}\right)\right\}.$$

We will call this the trapezium volume approximation formula.

Example: Lake 1. Let the depth of the lake be given by $f(x, y) = k \sin x \sin y$ where k is a positive constant and $0 \leqslant x, y \leqslant \pi$ with distances in kilometres. A cross-section of the lake taken perpendicularly from the midpoint of a side will essentially look like part of the graph of $-\sin x$.

The actual volume of the water in the lake will be given by

$$V = \int_0^\pi \int_0^\pi k \sin x \sin y \, dx \, dy = \int_0^\pi 2k \sin y \, dy = 4k \text{ km}^3.$$

Ignoring the constant k until the end and taking $h = \frac{\pi}{6}$ gives the following table for the values of the depths.

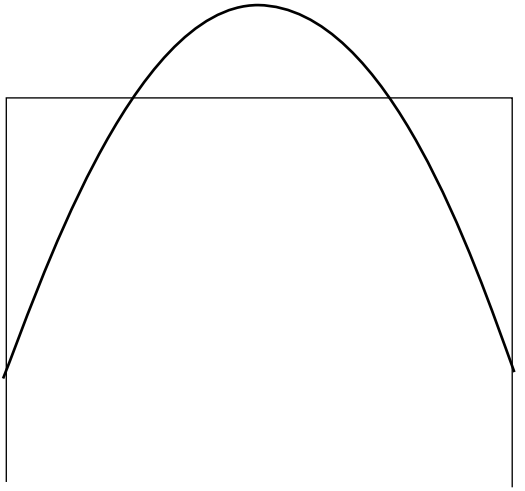
$y \backslash x$	0	$\frac{\pi}{6}$	$\frac{2\pi}{6}$	$\frac{3\pi}{6}$	$\frac{4\pi}{6}$	$\frac{5\pi}{6}$	π
0	0	0	0	0	0	0	0
$\frac{\pi}{6}$	0	$\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{4}$	0
$\frac{2\pi}{6}$	0	$\frac{\sqrt{3}}{4}$	$\frac{3}{4}$	$\frac{\sqrt{3}}{2}$	$\frac{3}{4}$	$\frac{\sqrt{3}}{4}$	0
$\frac{3\pi}{6}$	0	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	1	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$	0
$\frac{4\pi}{6}$	0	$\frac{\sqrt{3}}{4}$	$\frac{3}{4}$	$\frac{\sqrt{3}}{2}$	$\frac{3}{4}$	$\frac{\sqrt{3}}{4}$	0
$\frac{5\pi}{6}$	0	$\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{4}$	0
π	0	0	0	0	0	0	0

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Applying the Trapezium volume formula with the appropriate coefficients gives $V_T = 3.818k$ to 4 significant figures.

This underestimates (as expected from the curvature) the true volume by $0.182k$ (3sf) and has an absolute percentage error of 4.55%.

Example: Lake 2. This lake is deepest near the perimeter especially the corners and has an island in the middle. Its depth function is given by $f(x, y) = k(x^2 + y^2 - 1)$ for $-2 \leqslant x, y \leqslant 2$ where k is a positive constant and lengths are in kilometres. The negative values of $f(x, y)$ indicate dry land sticking up above the surface of the lake. This example will demonstrate the technique of changing negative readings to 0. A cross-section of the lake taken perpendicularly from the midpoint of a side will look as shown below.



Cross section of Lake 2

Now $\int_{-2}^{2}\int_{-2}^{2} k(x^2 + y^2 - 1)\,dx\,dy = \int_{-2}^{2} k\left(\frac{4}{3} + 4y^2\right)dy = \frac{80}{3}k$.

However this double integral will combine the volume of the water with the volume of the earth on the circular island that is above the water level of the lake, with this volume of earth being treated as negative. This volume of earth will be $k\int_0^{2\pi}\int_0^1 (r^2 - 1)r\,dr\,d\theta = k\int_0^{2\pi} -\frac{1}{4}d\theta = -\frac{\pi}{2}k$.

Hence the exact volume of water in the lake will be $k\left(\frac{80}{3} + \frac{\pi}{2}\right) = 28.237\ \text{km}^3$ (5sf). Ignoring the constant k until the end and taking $h = \frac{1}{2}$ gives the following table for the values of the depths, with those that are negative indicated that they will be taken as 0.

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$y\backslash x$	-2	$-\frac{3}{2}$	-1	$-\frac{1}{2}$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2
-2	7	$\frac{21}{4}$	4	$\frac{13}{4}$	3	$\frac{13}{4}$	4	$\frac{21}{4}$	7
$-\frac{3}{2}$	$\frac{21}{4}$	$\frac{14}{4}$	$\frac{9}{4}$	$\frac{6}{4}$	$\frac{5}{4}$	$\frac{6}{4}$	$\frac{9}{4}$	$\frac{14}{4}$	$\frac{21}{4}$
-1	4	$\frac{9}{4}$	1	$\frac{1}{4}$	0	$\frac{1}{4}$	1	$\frac{9}{4}$	4
$-\frac{1}{2}$	$\frac{13}{4}$	$\frac{6}{4}$	$\frac{1}{4}$	$-\frac{1}{2}\to 0$	$-\frac{3}{4}\to 0$	$-\frac{1}{2}\to 0$	$\frac{1}{4}$	$\frac{6}{4}$	$\frac{13}{4}$
0	3	$\frac{5}{4}$	0	$-\frac{3}{4}\to 0$	$-1\to 0$	$-\frac{3}{4}\to 0$	0	$\frac{5}{4}$	3
$\frac{1}{2}$	$\frac{13}{4}$	$\frac{6}{4}$	$\frac{1}{4}$	$-\frac{1}{2}\to 0$	$-\frac{3}{4}\to 0$	$-\frac{1}{2}\to 0$	$\frac{1}{4}$	$\frac{6}{4}$	$\frac{13}{4}$
1	4	$\frac{9}{4}$	1	$\frac{1}{4}$	0	$\frac{1}{4}$	1	$\frac{9}{4}$	4
$\frac{3}{2}$	$\frac{21}{4}$	$\frac{14}{4}$	$\frac{9}{4}$	$\frac{6}{4}$	$\frac{5}{4}$	$\frac{6}{4}$	$\frac{9}{4}$	$\frac{14}{4}$	$\frac{21}{4}$
2	7	$\frac{21}{4}$	4	$\frac{13}{4}$	3	$\frac{13}{4}$	4	$\frac{21}{4}$	7

Applying the trapezium volume formula, with the appropriate coefficients and negative values sent to 0 gives $V_T = 29.5k$. Note that with this method it does not matter where the origin is (here it is in the middle not at a corner of the grid) as we have the volume below any grid square just in terms of f values.

This overestimates (as expected) the true volume by $1.26k$ (3sf) and has an absolute percentage error of 4.47%.

To emulate the derivation of Simpson's rule we will next approximate $f(x)$ by the function

$$f_S(x, y) = a + bx + cx^2 + dy + fxy + gx^2y + ky^2 + lxy^2 + mx^2y^2$$

which is only of degree two in either x or y. We will consider the volume generated by this function on four grid square with coordinates given by $(0,0), (0,-h), (0,h), (-h,0), (h,0), (h,h), (-h,h), (h,-h), (-h.-h)$. These four grid squares are representative of any other four grid square but just keep the algebra simpler. In this case we will require both n_1 and n_2 to be even. The volume given by this function on these four grid squares will be

$$\begin{aligned} V_s &= \int_{-h}^{h}\int_{-h}^{h}\left(a + bx + cx^2 + dy + fxy + gx^2y + ky^2 + lxy^2 + mx^2y^2\right)dx\,dy \\ &= \int_{-h}^{h}\left(2ah + \frac{2ch^3}{3} + 2dhy + \frac{2gh^3y}{3} + 2khy^2 + \frac{2mh^3y^2}{3}\right)dy \\ &= 4ah^2 + \frac{4ch^4}{3} + \frac{4kh^4}{3} + \frac{4mh^6}{9} = \frac{h^2}{9}\left(36a + 12ch^2 + 12kh^2 + 4mh^2\right). \quad (2) \end{aligned}$$

Now we have

$f_{0,0} = a, f_{0,-1} = a - dh + kh^2, f_{0,1} = a + dh + kh^2, f_{-1,0} = a - bh + ch^2$

$f_{1,0} = a + bh + ch^2, f_{1,1} = a + bh + ch^2 + dh + fh^2 + gh^3 + kh^2 + lh^3 + mh^4,$

$f_{-1,1} = a - bh + ch^2 + dh - fh^2 + gh^3 + kh^2 - lh^3 + mh^4,$

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$f_{1,-1} = a + bh + ch^2 - dh - fh^2 - gh^3 + kh^2 + lh^3 + mh^4,$
$f_{-1,-1} = a - bh + ch^2 - dh + fh^2 - gh^3 + kh^2 - lh^3 + mh^4$
giving $f_{0,-1} + f_{0,1} + f_{-1,0} + f_{1,0} = 4a + 2(c + k)h^2$ and
$f_{1,1} + f_{-1,1} + f_{1,-1} + f_{-1,-1} = 4a + 2(c + k)h^2 + 4mh^4$ as the odd powers of h cancel out. So eliminating a, c, k, m from (2) we have

$$V_S = \frac{h^2}{9}\left(f_{1,1} + f_{-1,1} + f_{1,-1} + f_{-1,-1} + 4\left(f_{0,-1} + f_{0,1} + f_{-1,0} + f_{1,0}\right) + 16f_{0,0}\right).$$

This result has some symmetry and fits with a dimensions check. A similar result can be obtained for any other block of four grid squares. So an approximation for V will be

$$\frac{h^2}{9}\left(\text{a linear combination of the depths at the gridpoints}\right.$$

Considering a tabular display of depths the first row ($i = 0$) and the last row ($i = n_1$) will be entered with the coefficients following the pattern

1 4 2 4 2 4 … 4 2 4 1

Rows with i odd will be entered with the coefficient following the pattern

4 16 8 16 8 16 … 16 8 16 4

Rows with i even but $i \neq 0$, $i \neq n_1$ will be entered with the coefficient following the pattern

2 8 4 8 4 8 … 8 4 8 2

We will call this the Simpson volume approximation formula.

Example: Lake 1. The information and table for Lake 1 is given earlier. Applying the Simpson volume formula with the appropriate coefficients gives $V_S = 4.00345k$ (6sf).

This overestimates the true volume by 0.00345 (3sf) and has an absolute percentage error of 0.086%.

Example: Lake 2. The information and table for Lake 2 is given earlier. Applying the Simpson volume formula with the appropriate coefficients and negative values sent to 0 gives $V_S = \frac{85}{3}k = 28.3333k$.

This overestimates the true volume by $0.0957k$ (4sf) and has an absolute percentage error of 0.34%.

We will now consider the order of the trapezium volume approximation formula. Again we will work over the same grid square as before to keep the algebra simpler. We will assume that $f(x, y)$ is a well-behaved, continuous function and that all its partial derivatives exist over the interior surface of the lake. (We are not too concerned about the function on dry land or at the water/land boundary where there could be large drops). To keep the notation manageable we will use f to represent $f(0,0)$ and f_x to

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represent $\frac{\partial f}{\partial x}$ evaluated at (0,0) and so, for example, f_{yy} represents $\frac{\partial^2 f}{\partial y^2}$ evaluated at (0,0). The Maclaurin expansion for the function of two variables $f(x, y)$ will be

$$f(x, y) = f + xf_x + yf_y + \frac{1}{2!}\left(x^2 f_{xx} + 2xyf_{xy} + y^2 f_{yy}\right) + \dots .$$

Hence over the one grid square

$$\begin{aligned} V &= \int_0^h \int_0^h \left(f + xf_x + yf_y + \frac{1}{2}\left(x^2 f_{xx} + 2xyf_{xy} + y^2 f_{yy}\right) + \dots\right) dx\, dy \\ &= \int_0^h \left(hf + \frac{h^2}{2} f_x + hyf_y + \frac{h^3}{6} f_{xx} + \frac{hy^2}{2} f_{xy} + \frac{hy^2}{2} f_{yy} + \dots\right) dy \\ &= h^2 f + \frac{h^3}{2} f_x + \frac{h^3}{2} f_y + \frac{h^4}{6} f_{xx} + \frac{h^4}{4} f_{xy} + \frac{h^4}{6} f_{yy} + \text{higher terms in } h. \quad (3) \end{aligned}$$

We will compare this with $V_T = \frac{h^2}{4}\left(f_{0,0} + f_{0,1} + f_{1,0} + f_{1,1}\right)$, which is equal to

$$\begin{aligned} &\frac{h^2}{4}\left(f + \left(f + hf_y + \frac{h^2}{2} f_{yy} \dots\right) + \left(f + hf_x + \frac{h^2}{2} f_{xx} \dots\right) + \left(f + hf_x + hf_y + \frac{h^2}{2} f_{xx} + h^2 f_{xy} + \frac{h^2}{2} f_{yy} \dots\right)\right) \\ &= h^2 f + \frac{h^3}{2} f_x + \frac{h^3}{2} f_y + \frac{h^4}{2} f_{xx} + \frac{h^4}{4} f_{xx} + \frac{h^4}{4} f_{xy} + \text{higher terms in } h. \quad (4) \end{aligned}$$

Comparing (3) and (4) and choosing h small enough that the other terms can be neglected in comparison the error term is $\frac{h^4}{12}\left|f_{xx} + f_{yy}\right|$. There are $n_1 n_2$ such grid squares and $n_1 = \frac{l_1}{h}$, $n_2 = \frac{l_2}{h}$ giving the total error term as $\frac{l_1 l_2}{12} \max\left|f_{xx} + f_{yy}\right| h^2$ where now $f_{xx} + f_{yy}$ is used to represent the value of these partial derivatives over the whole surface of the lake. This error term shows that this rule is of second order, as is the usual trapezium rule and the format of the error term is very reminiscent of that of the error term in the usual trapezium rule. The error term confirms that if $f(x, y) = a + bx + cy + dxy$ then no error would be made and this includes the case when the bottom of the lake is a plane with equation of $f(x, y) = a + bx + cy$. At first sight it seems useful that if h was reduced by a factor of $\frac{1}{2}$ then the error would decrease by a factor of $\frac{1}{4}$, but originally the scientists had $(n_1 + 1)(n_2 + 1)$ readings to take, whereas reducing h by a factor of $\frac{1}{2}$ gives them $(2n_1 + 1)(2n_2 + 1)$ readings to take. As this is essentially four times as many readings they perhaps might not be too convinced about the usefulness.

Example: Lake 1. Here $f_{xx} + f_{yy} = -2k \sin x \sin y$ and $-2 \sin x \sin y$ lies in the set $[-1,0]$ for $0 \leqslant x, y \leqslant \pi$ and so the negative sign agrees with the underestimation. An upper bound for the absolute error would be $\frac{\pi^2}{12}\left(\frac{\pi}{6}\right)^2 \times 2k = 0.451k$ which also fits with the actual error.

Example: Lake 2. In this case the error term will not be looked at due to a slight problem with its derivation. It was assumed that the depth function was well-behaved. Because the negative values are changed to 0 then at the

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circumference of the island, although the new depth function will still be continuous, it will not be smooth at this boundary.

The order of the Simpson volume approximation formula could be found in a similar way. The comparison calculation is done over four grid squares and extra terms are taken in the Maclaurin expansion for the function of two variables. If this is done then the total error term comes out as $\frac{l_1 l_2}{180} \max \left| f_{xxxx} + f_{yyyy} \right| h^4$ where now $f_{xxxx} + f_{yyyy}$ is used to represent the value of these partial derivatives over the whole surface of the lake. This error term pleasingly shows that this rule is of order 4 as is the usual Simpson rule and the format of the error term is very reminiscent of that of the error term in the usual Simpson rule. The partial derivatives in this error term being of order 4 shows that if $f(x, y)$ is a polynomial in x and y where the degree of both x and y is smaller or equal to 3 then this method will not have any error. This is an extra bonus as the method was devised by fitting quadratics in x and y, and is again reminiscent of the usual Simpson's rule.

Example: Lake 1. Here $f_{xxxx} + f_{yyyy} = 2k \sin x \sin y$ and $2 \sin x \sin y$ lies in the set $[0, 2]$ for $0 \leqslant x, y \leqslant \pi$ and so the positive sign agrees with the overestimation. An upper bound for the absolute error would be $\frac{\pi^2}{180} \left(\frac{\pi}{6}\right)^4 \times 2k = 0.00824k$ which also fits with the actual error.

Example: Lake 2. Again here the error term will not be considered for the depth function with the 0 replacements, for the reasons explained before. If the table is used with the initial values (including the negative ones) then the exact value of $\frac{80}{3}$ will be obtained since $f_{xxxx} + f_{yyyy} = 0$ for this function with the highest power of x or y being 2. It is interesting to note that the value of $\frac{80}{3} + \frac{\pi}{2}$ can never be obtained exactly, as it is an irrational number and, with this example, no matter how small the value of h is taken as, the Simpson volume formula must produce a rational number.

If a trench parallel to the x-axis of width one grid square is considered with the depth function not altering as y varies then the trapezium volume approximation formula will generate the usual trapezium approximation for area, including the correct error term. Similarly if a trench parallel to the x-axis of width two grid squares is considered with the depth function not altering as y varies then the Simpson volume approximation formula will generate the usual Simpson approximation for area, including the correct error term.

These two approximations have problems if the lake profile has vertical cliffs or overhanging portions looking like the diagram below.



Overhang diagram

In these cases $f(x, y)$ would not be a function. However, in these two cases the contour method would also have similar problems.

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Lakes are just one of many possible applications that these 3D trapezium and Simpson rule approximations could be used for.

Reference

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