

# Numerical Analysis and Computing

Lecture Notes #09

— Numerical Integration and Differentiation —  
Multiple Integrals; Improper Integrals

Joe Mahaffy,  
(mahaffy@math.sdsu.edu)

Department of Mathematics  
Dynamical Systems Group  
Computational Sciences Research Center  
San Diego State University  
San Diego, CA 92182-7720

<http://www-rohan.sdsu.edu/~jmahaffy>

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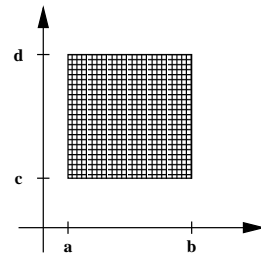


## The World is not One-Dimensional

Very few interesting problems are one-dimensional, so we need integration schemes for multiple integrals, *i.e.*

$$\mathcal{I} = \iint_R f(x, y) dx dy,$$

where  $R = \{(x, y) : x \in [a, b], y \in [c, d]\}$ .



**Good News:** The integration techniques we have developed previously can be adopted for multi-dimensional integration in a straight-forward way.

Composite Simpson's Rule (CSR) is our favorite integration scheme; we discuss multi-dimensional integration in that context.



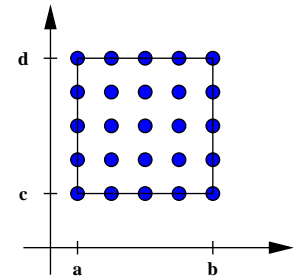
## Outline

- 1 Multiple Integrals
  - CSR in  $n$ -D
  - Non-Rectangular Domains
- 2 Improper Integrals
  - Calculus Treasures
  - Taylor Expansions... Surprise!



## Multi-Dimensional Composite Simpson's Rule

We divide the  $x$ -range  $[a, b]$  into an even number  $n_x$  of sub-intervals with nodes spaced  $h_x = (b - a)/n_x$  apart, and the  $y$ -range  $[c, d]$  into an even number  $n_y$  of sub-intervals with nodes spaced  $h_y = (d - c)/n_y$  apart.



We write

$$\mathcal{I} = \iint_R f(x, y) dx dy = \int_a^b \left[ \int_c^d f(x, y) dy \right] dx,$$

and first apply CSR to approximate the integration in  $y$  — treating  $x$  as a constant.



Composite Simpson's Rule in the  $y$ -coordinate

- ① Let  $y_j = c + jh_y$ ,  $j = 0, 1, \dots, n_y$ , then

$$\int_c^d f(x, y) dy = \frac{h_y}{3} \left[ f(x, y_0) - f(x, y_n) + \sum_{j=1}^{n_y/2} [2f(x, y_{2j}) + 4f(x, y_{2j-1})] \right] - \frac{(d-c)h_y^4}{180} \cdot \frac{\partial^4 f(x, \mu_y)}{\partial y^4},$$

for some  $\mu_y \in [c, d]$ .

- ② Then we apply the integral in the  $x$ -coordinate...

$$\begin{aligned} \int_a^b \int_c^d f(x, y) dy dx &= \frac{h_y}{3} \left[ \int_a^b f(x, y_0) dx - \int_a^b f(x, y_n) dx \right. \\ &\quad \left. + \sum_{j=1}^{n_y/2} \left[ 2 \int_a^b f(x, y_{2j}) dx + 4 \int_a^b f(x, y_{2j-1}) dx \right] \right] \\ &\quad - \frac{(d-c)h_y^4}{180} \int_a^b \frac{\partial^4 f(x, \mu_y)}{\partial y^4} dx, \end{aligned}$$

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## 2-Dimensional Composite Simpson's Rule — The Error

The error for the approximation is

$$E = -\frac{(b-a)(d-c)}{180} \left[ h_x^4 \frac{\partial^4 f}{\partial x^4}(\nu_x, \mu_x) + h_y^4 \frac{\partial^4 f}{\partial y^4}(\nu_y, \mu_y) \right]$$

for some  $(\nu_x, \mu_x), (\nu_y, \mu_y) \in R = [a, b] \times [c, d]$ .

**“Derivation of the error is left as an exercise for the interested reader...”**

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Apply Composite Simpson's Rule in the  $x$ -coordinate

Now, we “simply” apply CSR in the  $x$ -coordinate, for each integral in the expression...

$$\begin{aligned} \int_a^b \int_c^d f(x, y) dy dx &\approx \\ &\frac{h_x h_y}{9} \left\{ \left[ f(x_0, y_0) - f(x_n, y_0) + \sum_{i=1}^{n_x/2} (2f(x_{2i}, y_0) + 4f(x_{2i-1}, y_0)) \right] \right. \\ &\quad \left. - \left[ f(x_0, y_n) - f(x_n, y_n) + \sum_{i=1}^{n_x/2} (2f(x_{2i}, y_n) + 4f(x_{2i-1}, y_n)) \right] \right. \\ &\quad \left. + \sum_{j=1}^{n_y/2} \left[ 2 \left[ f(x_0, y_{2j}) - f(x_n, y_{2j}) + \sum_{i=1}^{n_x/2} (2f(x_{2i}, y_{2j}) + 4f(x_{2i-1}, y_{2j})) \right] \right. \right. \\ &\quad \left. \left. + 4 \left[ f(x_0, y_{2j-1}) - f(x_n, y_{2j-1}) + \sum_{i=1}^{n_x/2} (2f(x_{2i}, y_{2j-1}) + 4f(x_{2i-1}, y_{2j-1})) \right] \right] \right\} \end{aligned}$$

**This looks somewhat painful, but do not despair!!!** [First, a peek at the error...]

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## Building 2-D CSR in a Comprehensible Way?

Consider the tensor product of the  $x$ - and  $y$ -stencils for CSR with 2 sub-intervals:

$$\frac{h_x}{3} \begin{array}{|c|c|c|c|c|} \hline 1 & 4 & 2 & 4 & 1 \\ \hline \end{array} \otimes \frac{h_y}{3} \begin{array}{|c|} \hline 1 \\ 4 \\ 2 \\ 4 \\ 1 \\ \hline \end{array} = \frac{h_x h_y}{9} \begin{array}{|c|c|c|c|c|} \hline 1 & 4 & 2 & 4 & 1 \\ \hline 4 & 16 & 8 & 16 & 4 \\ \hline 2 & 8 & 4 & 8 & 2 \\ \hline 4 & 16 & 8 & 16 & 4 \\ \hline 1 & 4 & 2 & 4 & 1 \\ \hline \end{array}$$

Evaluate the function at the corresponding points, multiply by the above weights, and sum  $\Rightarrow$  2-D CSR.

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## Building 2-D CSR in a Comprehensible Way? — Example

$$\frac{9}{h_x h_y} \int_{x_0}^{x_4} \int_{y_0}^{y_4} f(x, y) dx dy \approx$$

$$1 \left[ f(x_0, y_0) + 4f(x_1, y_0) + 2f(x_2, y_0) + 4f(x_3, y_0) + f(x_4, y_0) \right] +$$

$$4 \left[ f(x_0, y_1) + 4f(x_1, y_1) + 2f(x_2, y_1) + 4f(x_3, y_1) + f(x_4, y_1) \right] +$$

$$2 \left[ f(x_0, y_2) + 4f(x_1, y_2) + 2f(x_2, y_2) + 4f(x_3, y_2) + f(x_4, y_2) \right] +$$

$$4 \left[ f(x_0, y_3) + 4f(x_1, y_3) + 2f(x_2, y_3) + 4f(x_3, y_3) + f(x_4, y_3) \right] +$$

$$1 \left[ f(x_0, y_4) + 4f(x_1, y_4) + 2f(x_2, y_4) + 4f(x_3, y_4) + f(x_4, y_4) \right]$$

$$h_x = \frac{x_4 - x_0}{4}, \quad h_y = \frac{y_4 - y_0}{4}.$$

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## Integrating Outside the Box

The integration schemes we have discussed so far only works for rectangular regions  $[a, b] \times [c, d]$ ...

In calculus we compute integrals of this form:

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y) dy dx$$

We can modify our integration schemes to deal with this type of integrals.

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## Building Higher-Dimensional Schemes

Using the same strategy, we can build a 3-D CSR-scheme

$$\text{CSR}_{xyz} = \text{CSR}_x \otimes \text{CSR}_y \otimes \text{CSR}_z.$$

There's nothing unique about the usage of CSR. The same idea can be used to build higher dimensional Gaussian Quadrature schemes. If we have the stencils for the one-dimensional (Composite) Gaussian Quadrature schemes in the  $x$ -,  $y$ - and  $z$ -directions ( $\text{GQ}_x$ ,  $\text{GQ}_y$ ,  $\text{GQ}_z$ ):

$$\text{GQ}_{xyz} = \text{GQ}_x \otimes \text{GQ}_y \otimes \text{GQ}_z.$$

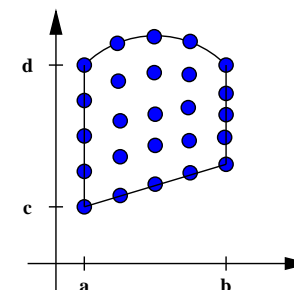
If you're really twisted you could use different schemes in the different coordinate directions, *i.e.*

$$\text{NUMINT}_{xyz} = \text{CSR}_x \otimes \text{GQ}_y \otimes \text{Romberg}_z.$$

Needless to say, the error terms would get really "interesting."

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## Dealing with Variable Integration Limits



In order to numerically compute an integral of this type

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y) dy dx$$

we are going to use CSR with a fixed step size  $h_x = (b - a)/n_x$  in the  $x$ -direction, and variable step size  $h_y = (d(x) - c(x))/n_y$  in the  $y$ -direction.

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## Variable Integration Limits — Example

For simplicity we apply straight-up one-step SR to

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y) dy dx$$

and get

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y) dy dx \approx \frac{h_x}{3} \left\{ \frac{d(x_0)-c(x_0)}{6} \left[ f(x_0, c(x_0)) + 4f(x_0, \frac{c(x_0)+d(x_0)}{2}) + f(x_0, d(x_0)) \right] + \frac{4(d(x_1)-c(x_1))}{6} \left[ f(x_1, c(x_1)) + 4f(x_1, \frac{c(x_1)+d(x_1)}{2}) + f(x_1, d(x_1)) \right] + \frac{d(x_2)-c(x_2)}{6} \left[ f(x_2, c(x_2)) + 4f(x_2, \frac{c(x_2)+d(x_2)}{2}) + f(x_2, d(x_2)) \right] \right\},$$

$$\text{where } x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b.$$

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## Algorithm: Variable Limits Double Integral using CSR

## Algorithm: Variable Limits Double Integral – CSR

```
[1] hx = (b-a)/n, ENDPTS=0, EVENPTS=0, ODDPTS=0
[2] FOR i = 0, 1, ..., n                                % CSR in x
    x = a + i*hx
    k1 = f(x, c(x)) + f(x, d(x))                        % End terms
    k2 = 0                                                % Even terms
    k3 = 0                                                % Odd terms
    hy = (d(x)-c(x))/n
    FOR j = 1, 2, ..., (m-1)
        y = c(x)+j*hy
        Q = f(x, y)
        IF j EVEN: k2 += Q, ELSE: k3 += Q
    END-FOR-j
    L = hy*(k1 + 2*k2 + 4*k3)/3;
    IF i is 0 OR n: ENDPTS += L
    ELSEIF i EVEN:  EVENPTS += L
    ELSEIF i ODD:   ODDPTS  += L
END-FOR-i
INTAPPROX = hx*(ENDPTS+2*EVENPTS+4*ODDPTS)/3
```

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## Variable Integration Limits

We can imagine how to extend to multiple dimensions, *i.e.*

$$\int_a^b \int_{c(x)}^{d(x)} \int_{e(x,y)}^{f(x,y)} g(x, y, z) dz dy dx.$$

Again, there nothing special about Simpson's Rule — we can attack variable integration limits with Gaussian Quadrature, Trapezoidal Rule, or Boole's Rule...

Note that there is nothing stopping us from using adaptive schemes to find the integrals... but the complexity of the code grows!

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## Improper Integrals — Introduction

"Improper" integrals:

[1] Integrals over infinite intervals

$$\int_a^\infty f(x) dx.$$

[2] Integrals with unbounded functions

$$\int_a^b \frac{f(x)}{(x-a)^p} dx.$$

**Note:** We can always transform [1]  $\rightarrow$  [2]

$$\int_a^\infty f(x) dx = \left\{ \begin{array}{l} t = x^{-1} \\ dt = -x^{-2} dx \end{array} \right\} = \int_{1/a}^0 -t^{-2} f(t^{-1}) dt$$

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## More Forgotten Calculus

The integral

$$\int_a^b \frac{dx}{(x-a)^p}$$

converges if and only if  $p \in (-\infty, 1)$ , and

$$\int_a^b \frac{dx}{(x-a)^p} = \frac{(b-a)^{1-p}}{1-p}.$$

If  $f(x)$  can be written on the form

$$f(x) = \frac{g(x)}{(x-a)^p}, \quad p \in (-\infty, 1), \quad g \in C[a, b]$$

then the improper integral

$$\int_a^b f(x) dx, \text{ exists.}$$

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## Splitting the Integrand using Taylor Expansions

II/II

If we let

$$\int_a^b f(x) dx \approx \sum_{k=0}^d \frac{g^{(k)}(a)}{k!(k+1-p)} (b-a)^{k+1-p},$$

then the approximation error is bounded by:

$$\begin{aligned} \int_a^b \frac{g(x) - P_d(x)}{(x-a)^p} dx &= \int_a^b \frac{R_d(x)}{(x-a)^p} dx = \int_a^b \frac{g^{(d+1)}(\xi(x))(x-a)^{d+1}}{(k+1)!(x-a)^p} dx \\ &\leq \frac{1}{(k+1)!} \max_{x \in [a,b]} |g^{(d+1)}(x)| \int_a^b (x-a)^{d+1-p} dx \\ &= \frac{g^{(d+1)}(\xi)}{(k+1)!(d+2-p)} (b-a)^{d+2-p}. \end{aligned}$$

What if we want to do better?

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## Splitting the Integrand using Taylor Expansions

I/II

Assuming that  $g \in C^{d+1}[a, b]$ , for some  $d \in \mathbb{Z}^+$ , the Taylor polynomial of degree  $d$  is

$$P_d(x) = \sum_{k=0}^d \frac{g^{(k)}(a)(x-a)^k}{k!}.$$

We can now write

$$\int_a^b f(x) dx = \int_a^b \frac{g(x) - P_d(x)}{(x-a)^p} dx + \int_a^b \frac{P_d(x)}{(x-a)^p} dx,$$

where the last integral is easy to find, since  $P_d(x)$  is a polynomial:

$$\sum_{k=0}^d \int_a^b \frac{g^{(k)}(a)}{k!} (x-a)^{k-p} dx = \sum_{k=0}^d \frac{g^{(k)}(a)}{k!(k+1-p)} (b-a)^{k+1-p}$$

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## Numerical Approximation of the Remainder Term

To get a more accurate approximation to the integral, we compute the numerical approximation of the remainder term:

$$\int_a^b \frac{g(x) - P_d(x)}{(x-a)^p} dx.$$

**Define:** (Remove the singularity)

$$G(x) = \begin{cases} \frac{g(x) - P_d(x)}{(x-a)^p} & x \in (a, b] \\ 0 & x = a. \end{cases}$$

**Apply:** Composite Simpson's Rule

$$\int_a^b G(x) dx \approx \frac{h}{3} \left[ G(x_0) - G(x_n) + \sum_{j=1}^{n/2} \left[ 4G(x_{2j-1}) + 2G(x_{2j}) \right] \right].$$

Add the CSR-approximation to  $\sum_{k=0}^d \frac{g^{(k)}(a)}{k!(k+1-p)} (b-a)^{k+1-p}$ .

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## Example#1

I/III

We want to compute

$$\int_0^1 \frac{e^x}{x^{1/2}} dx.$$

The fourth order Taylor polynomial is

$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24},$$

so

$$\begin{aligned} \int_0^1 \frac{P_4(x)}{x^{1/2}} dx &= \int_0^1 x^{-1/2} + x^{1/2} + \frac{x^{3/2}}{2} + \frac{x^{5/2}}{6} + \frac{x^{7/2}}{24} dx \\ &= \frac{2}{1} + \frac{2}{3} + \frac{2}{2 \cdot 5} + \frac{2}{6 \cdot 7} + \frac{2}{24 \cdot 9} \approx 2.923544974 \end{aligned}$$

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## Example#1

III/III

Since  $|G^{(4)}(x)| < 1$  on  $(0, 1]$ , the error from CSR is bounded by

$$\frac{1}{180} \cdot \frac{1}{4^4} = 0.0000217.$$

The error bound for the Taylor-only approximation is bounded by

$$\frac{1}{5! \cdot 5.5} = 0.00151515$$

If, instead of adding the CSR-approximation of  $\int G(x) dx$ , we used  $P_5(x)$ , the error bound for that Taylor-only approximation would be

$$\frac{1}{6! \cdot 6.5} = 0.00021044.$$

The  $P_6(x)$ -only-error is comparable with the  $P_4(x)$ +CSR-error:

$$\frac{1}{7! \cdot 7.5} = 0.000026455.$$

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## Example#1

II/III

Next, we apply CSR with  $h = 1/4$  to  $\int_0^1 G(x) dx$ , where

$$G(x) = \begin{cases} \frac{e^x - P_4(x)}{x^{1/2}} & x \in (0, 1] \\ 0 & x = 0. \end{cases}$$

$$\begin{aligned} \int_0^1 G(x) dx &\approx \frac{1}{4 \cdot 3} \left[ 0 + 4 \cdot 0.0000170 + 2 \cdot 0.00413 + 4 \cdot 0.0026026 \right. \\ &\quad \left. + 0.0099485 \right] = 0.0017691. \end{aligned}$$

Hence,

Result

$$\int_0^1 \frac{e^x}{x^{1/2}} dx \approx 2.923544974 + 0.0017691 = 2.9253141$$

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## Example#2

I/II

We are going to approximate the integral

$$\int_1^\infty \frac{1}{x^{3/2}} \sin\left(\frac{1}{x}\right) dx.$$

A quick change of variables  $t = x^{-1}$  gives us

$$\int_0^1 t^{-1/2} \sin(t) dt.$$

The sixth Taylor polynomial  $P_6(t)$  for  $\sin(t)$  about  $t = 0$  is

$$P_6(t) = t - \frac{1}{6}t^3 + \frac{1}{120}t^5, \quad |R_6(t)| \leq \frac{1}{7!} = 0.00019841$$

$$\begin{aligned} \int_0^1 t^{-1/2} P_6(t) dt &= \int_0^1 t^{1/2} - \frac{1}{6}t^{5/2} + \frac{1}{120}t^{9/2} dt \\ &= \frac{2}{3} - \frac{2}{7 \cdot 6} + \frac{2}{11 \cdot 120} = 0.62056277 \end{aligned}$$

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## Example#2

11/11

We define

$$G(t) = \begin{cases} \frac{\sin(t) - P_6(t)}{t^{1/2}} & t \in (0, 1] \\ 0 & t = 0, \end{cases}$$

and apply CSR with  $h = 1/32$  to  $\int_0^1 G(t) dt$  to get

## Result

$$\int_1^\infty \frac{1}{x^{3/2}} \sin\left(\frac{1}{x}\right) dx$$
$$\approx 0.62056277 - 0.0000261672790305 = 0.62053660 \dots$$

which is accurate to within  $\sim 10^{-8}$ .

