Numerical Analysis and Computing

Lecture Notes #09

— Numerical Integration and Differentiation —

Multiple Integrals; Improper Integrals

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Outline

1. Multiple Integrals
   - CSR in n-D
   - Non-Rectangular Domains

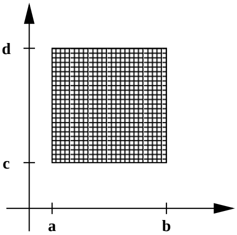
2. Improper Integrals
   - Calculus Treasures
   - Taylor Expansions... Surprise!

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

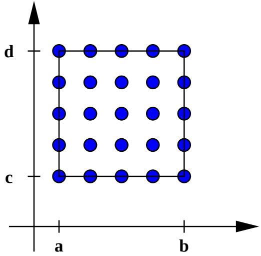


Good News: The integration techniques we have developed previously can be adopted for multi-dimensional integration in a straight-forward way.

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

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

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

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

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

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

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

Apply Composite Simpson's Rule in the x-coordinate

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

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$$\int_a^b \int_c^d f(x,y)\,dy\,dx \approx$$

$$\frac{h_x h_y}{9}\Bigg\{\Bigg[f(x_0,y_0) - f(x_n,y_0) + \sum_{i=1}^{n_x/2}\Big(2f(x_{2i},y_0) + 4f(x_{2i-1},y_0)\Big)\Bigg]$$

$$-\Bigg[f(x_0,y_n) - f(x_n,y_n) + \sum_{i=1}^{n_x/2}\Big(2f(x_{2i},y_n) + 4f(x_{2i-1},y_n)\Big)\Bigg]$$

$$+\sum_{j=1}^{n_y/2}\Bigg[2\Bigg[f(x_0,y_{2j}) - f(x_n,y_{2j}) + \sum_{i=1}^{n_x/2}\Big(2f(x_{2i},y_{2j}) + 4f(x_{2i-1},y_{2j})\Big)\Bigg]$$

$$+4\Bigg[f(x_0,y_{2j-1}) - f(x_n,y_{2j-1}) + \sum_{i=1}^{n_x/2}\Big(2f(x_{2i},y_{2j-1}) + 4f(x_{2i-1},y_{2j-1})\Big)\Bigg]\Bigg]\Bigg\}$$

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

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..."

Building 2-D CSR in a Comprehensible Way?

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

$$\frac{h_x}{3}\quad \boxed{1}-\boxed{4}-\boxed{2}-\boxed{4}-\boxed{1} \quad \otimes \quad \frac{h_y}{3}\ \begin{array}{c}\boxed{1}\\ | \\ \boxed{4}\\ | \\ \boxed{2}\\ | \\ \boxed{4}\\ | \\ \boxed{1}\end{array} \quad =$$

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$$\frac{h_x}{3}\begin{bmatrix} 1 & 4 & 2 & 4 & 1 \end{bmatrix} \otimes \frac{h_y}{3}\begin{bmatrix} 1 \\ 4 \\ 2 \\ 4 \\ 1 \end{bmatrix} = \frac{h_x h_y}{9}\begin{bmatrix} 1 & 4 & 2 & 4 & 1 \\ 4 & 16 & 8 & 16 & 4 \\ 2 & 8 & 4 & 8 & 2 \\ 4 & 16 & 8 & 16 & 4 \\ 1 & 4 & 2 & 4 & 1 \end{bmatrix}$$

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

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

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

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

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

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

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

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

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

Building Higher-Dimensional Schemes

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

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

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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 (GQ_x, GQ_y, GQ_z):

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

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

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

Integrating Outside the Box

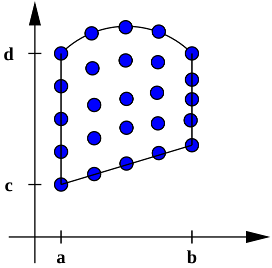
The integration schemes we have discussed so far only works for rectangular regions $[a, b] \times [c, d]$...

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.

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.

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

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

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

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!

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
```

Improper Integrals — Introduction

"Improper" integrals:

[1] Integrals over infinite intervals

$$\int_a^{\infty} f(x)\,dx.$$

[2] Integrals with unbounded functions

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

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

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

More Forgotten Calculus

The integral

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

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

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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

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

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

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

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We can now write

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

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

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

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:

$$\int_a^b \frac{g(x)-P_d(x)}{(x-a)^p}\,dx = \int_a^b \frac{R_d(x)}{(x-a)^p}\,dx = \int_a^b \frac{g^{(d+1)}(\xi(x))(x-a)^{d+1}}{(k+1)!(x-a)^p}\,dx$$

$$\leq \frac{1}{(k+1)!}\max_{x\in[a,b]}|g^{(d+1)}(x)|\int_a^b (x-a)^{d+1-p}\,dx$$

$$= \mathbf{\frac{g^{(d+1)}(\xi)}{(k+1)!\,(d+2-p)}(b-a)^{d+2-p}}.$$

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$$= \frac{\mathbf{g^{(d+1)}(\xi)}}{\mathbf{(k+1)!\,(d+2-p)}}\mathbf{(b-a)^{d+2-p}}.$$

What if we want to do better?

Numerical Approximation of the Remainder Term

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

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

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Define: (Remove the singularity)

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

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Apply: Composite Simpson's Rule

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

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

Example#1 I/III

We want to compute

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

The fourth order Taylor polynomial is

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

Example#1

I/III

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The fourth order Taylor polynomial is
$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24},$$
so
$$\int_0^1 \frac{P_4(x)}{x^{1/2}}\,dx = \int_0^1 x^{-1/2} + x^{1/2} + \frac{x^{3/2}}{2} + \frac{x^{5/2}}{6} + \frac{x^{7/2}}{24}\,dx$$
$$= \frac{2}{1} + \frac{2}{3} + \frac{2}{2\cdot 5} + \frac{2}{6\cdot 7} + \frac{2}{24\cdot 9} \approx 2.923544974$$

Example#1 II/III

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

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

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$$\int_0^1 G(x)\,dx \approx \frac{1}{4 \cdot 3}\Big[0 + 4 \cdot 0.0000170 + 2 \cdot 0.00413 + 4 \cdot 0.0026026$$

$$+0.0099485\Big] = 0.0017691.$$

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Hence,

Result

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

Example#1 III/III

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

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

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

Example#2

We are going to approximate the integral

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

Example#2 I/II

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

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

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

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

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

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

$$\int_0^1 t^{-1/2} P_6(t)\, dt = \int_0^1 t^{1/2} - \frac{1}{6}t^{5/2} + \frac{1}{120}t^{9/2}\, dt$$

$$= \frac{2}{3} - \frac{2}{7 \cdot 6} + \frac{2}{11 \cdot 120} = 0.62056277$$

Example#2 II/II

We define

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

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

Result

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

$$\approx 0.62056277 - 0.000026167279035 = 0.62053660\ldots$$

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