Numerical Integration and Differentiation

Multiple Integrals; Improper Integrals

Lecture Notes #9

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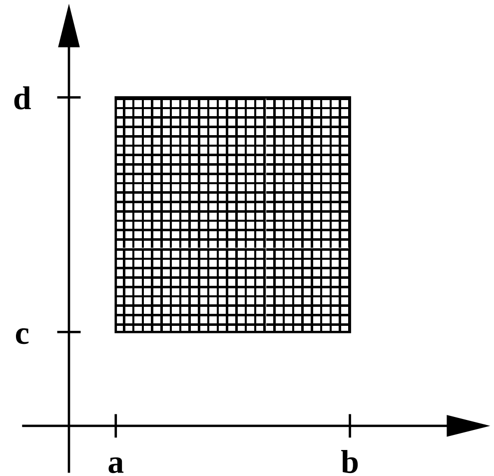
Very few interesting problems are one-dimensional, so we need integration schemes for multiple integrals, *i.e.*

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

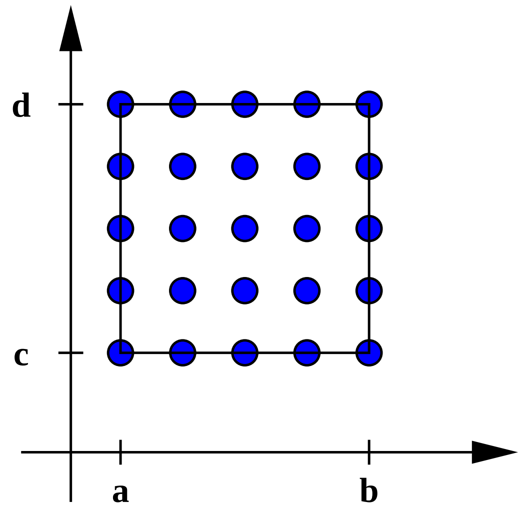


where $R = \{(x,y) : x \in [a,b],\ y \in [c,d]\}$.

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, so we will discuss multi-dimensional integration in that context.

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

Let $y_j = c + jh_y$, $j = 0, 1, \ldots, n_y$, 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 $\mu_y \in [c,d]$.

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

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

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!!!

2-Dimensional Composite Simpson's Rule — The Error

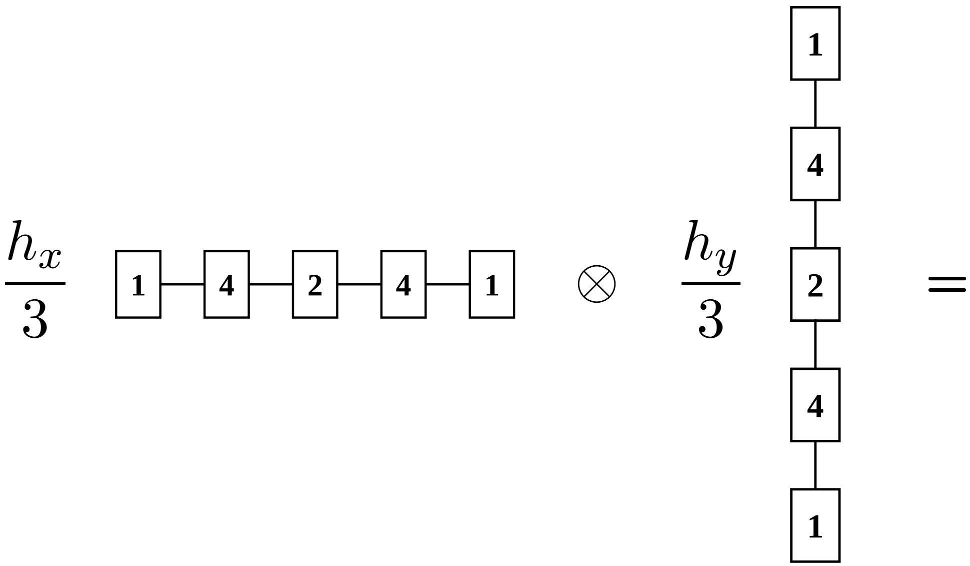
The error for the approximation is

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

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..."

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



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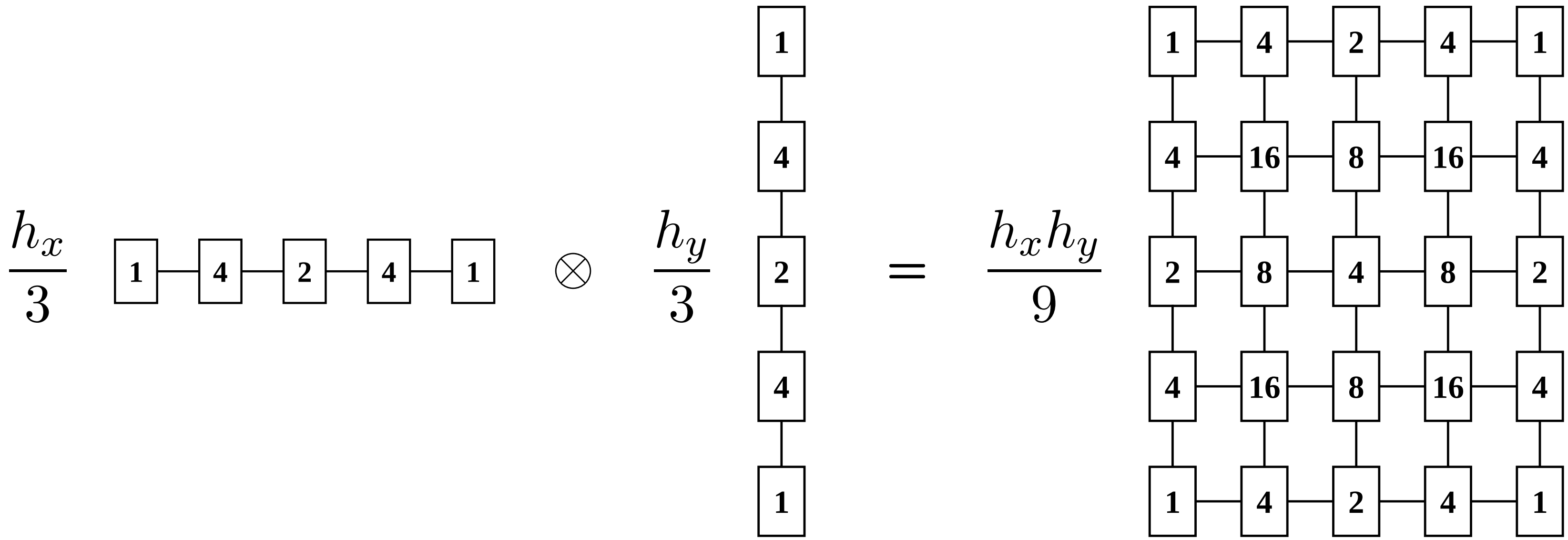

Consider the tensor product of the x- and y-stencils for CSR with 2 sub-intervals:

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

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

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

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

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

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

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

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

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

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

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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.*

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

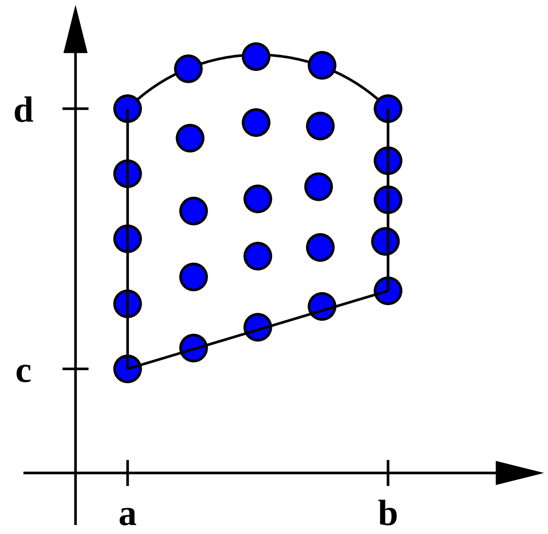
Needless to day, the error terms would get really *"interesting."*

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.



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.

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

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

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

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

```
[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:

[1] Integrals over infinite intervals

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

[2] Integrals with unbounded functions

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Note: We can always transform **[1]**→**[2]**

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

The integral

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

converges if and only if $p \in (0,1)$, and

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

$$f(x) = \frac{g(x)}{(x-a)^p}, \quad p \in (0,1), \quad g \in C[a,b]$$

then the improper integral

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

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

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

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

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

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:

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

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

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

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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:

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Define: (Remove the singularity)

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

We want to compute

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

The fourth order Taylor polynomial is

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so

$$\int_0^1 \frac{P_4(x)}{x^{1/2}}\,dx = \int_0^1 x^{-1/2} + x^{1/2} + \frac{x^{3/2}}{2} + \frac{x^{5/2}}{6} + \frac{x^{7/2}}{24}\,dx$$

$$= \frac{2}{1} + \frac{2}{3} + \frac{2}{2\cdot 5} + \frac{2}{6\cdot 7} + \frac{2}{24\cdot 9} \approx 2.923544974$$

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,

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

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

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

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

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

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

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

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

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

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

$$\approx \mathbf{0.62056277 - 0.000026167279030 5 = 0.62053660}$$

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