Indian Institute of Technology, Madras

Computational Tools: Algorithms, Data Structures and Programs - ID6105

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1 Problem 1

Function: $f(x,y) = 2xy^2 + 3e^{xy}$

Gradient:

$$\nabla f(x,y) = \begin{bmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2y^2 + 3ye^{xy} \\ 4xy + 3xe^{xy} \end{bmatrix}$$

Hessian:

$$H_f(x,y) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x^2} & \dfrac{\partial^2 f}{\partial x \partial y} \\ \dfrac{\partial^2 f}{\partial y \partial x} & \dfrac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 3y^2e^{xy} & 4y + 3e^{xy} + 3xye^{xy} \\ 4y + 3e^{xy} + 3xye^{xy} & 4x + 3x^2e^{xy} \end{bmatrix}$$

Function: $f(x,y,z) = x^2 + y^2 + 2z^2$

Gradient:

$$\nabla f(x,y,z) = \begin{bmatrix} 2x \\ 2y \\ 4z \end{bmatrix}$$

Hessian:

$$H_f(x,y,z) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

Function: $f(x,y) = \ln(x^2 + 2xy + 3y^2)$, let $g(x,y) = x^2 + 2xy + 3y^2$.

Gradient:

$$\nabla f(x,y) = \begin{bmatrix} \dfrac{2x + 2y}{g(x,y)} \\ \dfrac{2x + 6y}{g(x,y)} \end{bmatrix}$$

Hessian:

$$H_f(x,y) = \frac{1}{g(x,y)^2}\begin{bmatrix} 2g(x,y)-(2x+2y)^2 & 2g(x,y)-(2x+2y)(2x+6y) \\ 2g(x,y)-(2x+2y)(2x+6y) & 6g(x,y)-(2x+6y)^2 \end{bmatrix}$$

The second partial derivatives are,

$$f_{xx} = \frac{2g(x,y)-(2x+2y)^2}{g(x,y)^2},$$

$$f_{xy} = \frac{2g(x,y)-(2x+2y)(2x+6y)}{g(x,y)^2},$$

$$f_{yy} = \frac{6g(x,y)-(2x+6y)^2}{g(x,y)^2}$$

2 Problem 2

Code:

```python
import numpy as np

# Stopping criterion
def relative_change(x_new, x_old):
    return np.linalg.norm(x_new - x_old) / max(1.0, np.linalg.norm(x_old))

# Function: f(x, y) = (x-3)^2 + (y-2)^2
def f_a(v):
    x, y = v
    return (x - 3)**2 + (y - 2)**2

def grad_a(v):
    x, y = v
    return np.array([2*(x - 3), 2*(y - 2)])

def hess_a(v):
    return 2*np.eye(2)

# Function: f(x, y, z) = exp(-(x-5)^2 - (y-8)^2 - 2*(z-3)^2)
def f_b(v):
    x, y, z = v
    return np.exp(-((x - 5)**2 + (y - 8)**2 + 2*(z - 3)**2))

def grad_b(v):
    x, y, z = v
    c = f_b(v)
    return c * np.array([-2*(x - 5), -2*(y - 8), -4*(z - 3)])

def hess_b(v):
    x, y, z = v
    c = f_b(v)
    H = np.array([[-2, 0, 0], [0, -2, 0], [0, 0, -4]]) * c
    g = grad_b(v)
    return H + np.outer(g, np.array([(x - 5), (y - 8), 2*(z - 3)]))

# Function: f(x, y) = ln(x^2 + 2xy + 3y^2 - 4y + 3)
def f_c(v):
    x, y = v
    Q = x**2 + 2*x*y + 3*y**2 - 4*y + 3
```

```python
    return np.log(Q)

def grad_c(v):
    x, y = v
    Q = x**2 + 2*x*y + 3*y**2 - 4*y + 3
    return (1/Q) * np.array([2*x + 2*y, 2*x + 6*y - 4])

def hess_c(v):
    x, y = v
    Q = x**2 + 2*x*y + 3*y**2 - 4*y + 3
    gradQ = np.array([2*x + 2*y, 2*x + 6*y - 4])
    Hq = np.array([[2, 2], [2, 6]])
    return (1/Q)*Hq - (1/Q**2)*np.outer(gradQ, gradQ)

def steepest_method(f, grad, x0, ascent=False, lr=0.1, tol=0.01, max_iter=1000):
    x = np.array(x0, dtype=float)
    path = [x.copy()]
    for i in range(max_iter):
        g = grad(x)
        if ascent:
            x_new = x + lr * g
        else:
            x_new = x - lr * g
        path.append(x_new.copy())
        if relative_change(x_new, x) < tol:
            break
        x = x_new
    return x, f(x), len(path), np.array(path)

def newton_method(f, grad, hess, x0, ascent=False, tol=0.01, max_iter=100):
    x = np.array(x0, dtype=float)
    path = [x.copy()]
    for _ in range(max_iter):
        g = grad(x)
        H = hess(x)
        try:
            step = np.linalg.solve(H, g)
        except np.linalg.LinAlgError:
            step = np.linalg.lstsq(H, g, rcond=None)[0]
        if ascent:
            x_new = x + step
        else:
            x_new = x - step
        path.append(x_new.copy())
        if relative_change(x_new, x) < tol:
            break
        x = x_new
    return x, f(x), len(path), np.array(path)

x0_a = [1, 1]
res_a_sd = steepest_method(f_a, grad_a, x0_a, ascent=False, lr=0.25)
res_a_newton = newton_method(f_a, grad_a, hess_a, x0_a, ascent=False)

x0_b = [0, 0, 0]
res_b_sd = steepest_method(f_b, grad_b, x0_b, ascent=True, lr=0.01)
res_b_newton = newton_method(f_b, grad_b, hess_b, x0_b, ascent=True)

x0_c = [0, 0]
res_c_sd = steepest_method(f_c, grad_c, x0_c, ascent=False, lr=0.05)
res_c_newton = newton_method(f_c, grad_c, hess_c, x0_c, ascent=False)

# Results
```

```python
print("Problem (a): Quadratic bowl")
print("Steepest descent:", res_a_sd[0], " f =", res_a_sd[1], " Iter =", res_a_sd[2])
print("Newton's method :", res_a_newton[0], " f =", res_a_newton[1], " Iter =",
↪   res_a_newton[2])
print()

print("Problem (b): Gaussian peak")
print("Steepest ascent:", res_b_sd[0], " f =", res_b_sd[1], " Iter =", res_b_sd[2])
print("Newton's method:", res_b_newton[0], " f =", res_b_newton[1], " Iter =",
↪   res_b_newton[2])
print()

print("Problem (c): Log-quadratic valley")
print("Steepest descent:", res_c_sd[0], " f =", res_c_sd[1], " Iter =", res_c_sd[2])
print("Newton's method :", res_c_newton[0], " f =", res_c_newton[1], " Iter =",
↪   res_c_newton[2])
```

Output:

```
Problem (a): Quadratic bowl
Steepest descent: [2.9375  1.96875]  f = 0.0048828125  Iter = 7
Newton's method : [3. 2.]  f = 0.0  Iter = 3

Problem (b): Gaussian peak
Steepest ascent: [0. 0. 0.]  f = 3.392270193026015e-47  Iter = 2
Newton's method: [-2.9503714  -4.72059423 -1.77022284]  f = 3.231887011425879e-118
↪  Iter = 84

Problem (c): Log-quadratic valley
Steepest descent: [-0.81135203  0.92185695]  f = 0.024130512032747787  Iter = 43
Newton's method : [ 2.64277016e+30 -2.64277016e+30]  f = 140.79190810223392  Iter = 101
```

In case (a), the hessian is constant and hence, Newton's method determines the root in a minimal number of steps for quadratic functions. In case (b) both methods fail since the initial guess is relatively far from the actual peak. In case (c), Newton's method diverges (since the hessian is indefinite), while steepest descent converges to the solution slowly.

3 Problem 3

The integral,

$$I = \int_0^3 x^2 e^{2x} dx$$

Solving analytically (integration by parts),

$$I = \left[e^{2x} \left(\frac{x^2}{2} - \frac{x}{2} + \frac{1}{4} \right) \right]_0^3 \approx 1310.89357885$$

Code:

```python
import math

def f(x):
    return x**2 * math.exp(2*x)

I_exact = math.exp(6) * (9/2 - 3/2 + 1/4) - math.exp(0) * (0 - 0 + 1/4)
```

```python
def trapezoidal(a,b):
    return (b-a)/2.0 * (f(a) + f(b))

I_T = trapezoidal(0,3)
print("Trapezoidal Rule Approximation: ", I_T)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_T) / abs(I_exact))
print()

def trapezoidal_composite(a,b,n):
    h = (b - a) / n
    integral = 0.5 * (f(a) + f(b))
    for i in range(1, n):
        integral += f(a + i * h)
    integral *= h
    return integral

I_T_composite = trapezoidal_composite(0,3,2)
print("Composite Trapezoidal Rule Approximation (n=2): ", I_T_composite)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_T_composite) / abs(I_exact))
print()

I_T_composite = trapezoidal_composite(0,3,4)
print("Composite Trapezoidal Rule Approximation (n=4): ", I_T_composite)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_T_composite) / abs(I_exact))
print()

def simpsons_13(a,b):
    return (b - a) / 6.0 * (f(a) + 4.0 * f((a + b) / 2.0) + f(b))

I_S = simpsons_13(0,3)
print("Simpson's Rule Approximation: ", I_S)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_S) / abs(I_exact))
print()

def simpsons_composite(a,b,n):
    if n % 2 == 1:
        n += 1  # Make n even
    h = (b - a) / n
    integral = f(a) + f(b)
    for i in range(1, n, 2):
        integral += 4 * f(a + i * h)
    for i in range(2, n-1, 2):
        integral += 2 * f(a + i * h)
    integral *= h / 3
    return integral

I_S_composite = simpsons_composite(0,3,4)
print("Composite Simpson's Rule Approximation (n=4): ", I_S_composite)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_S_composite) / abs(I_exact))

def simpsons_38(a,b):
    return (3 * (b - a) / 8.0) * (f(a) + 3.0 * f(a + (b - a) / 3.0) + 3.0 * f(a + 2 *
     ↪  (b - a) / 3.0) + f(b))

I_S38 = simpsons_38(0,3)
print("\nSimpson's 3/8 Rule Approximation: ", I_S38)
```

```
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_S38) / abs(I_exact))
print()

def simpsons_38_composite(a,b,n):
    if n % 3 != 0:
        n += 3 - (n % 3)  # Make n a multiple of 3
    h = (b - a) / n
    integral = f(a) + f(b)
    for i in range(1, n, 3):
        integral += 3 * f(a + i * h)
    for i in range(2, n, 3):
        integral += 3 * f(a + i * h)
    for i in range(3, n-2, 3):
        integral += 2 * f(a + i * h)
    integral *= (3 * h / 8)
    return integral

I_S38_composite = simpsons_38_composite(0,3,5)
print("Composite Simpson's 3/8 Rule Approximation (n=5): ", I_S38_composite)
print("Exact Integral Value: ", I_exact)
print("Relative Error: ", abs(I_exact - I_S38_composite) / abs(I_exact))
```

Output:

```
Trapezoidal Rule Approximation:  5446.288712151924
Exact Integral Value:  1310.893578851389
Relative Error:  3.154638332216096

Composite Trapezoidal Rule Approximation (n=2):  2790.9330431917206
Exact Integral Value:  1310.893578851389
Relative Error:  1.1290309817804958

Composite Trapezoidal Rule Approximation (n=4):  1739.1410295790777
Exact Integral Value:  1310.893578851389
Relative Error:  0.32668361309918154

Simpson's Rule Approximation:  1905.8144868716524
Exact Integral Value:  1310.893578851389
Relative Error:  0.4538285316352955

Composite Simpson's Rule Approximation (n=4):  1388.543691708197
Exact Integral Value:  1310.893578851389
Relative Error:  0.059234490205410356

Simpson's 3/8 Rule Approximation:  4846.729623895281
Exact Integral Value:  1310.893578851389
Relative Error:  2.6972716184497663

Composite Simpson's 3/8 Rule Approximation (n=5):  1346.882713280276
Exact Integral Value:  1310.893578851389
Relative Error:  0.0274538948161
```

4 Problem 4

Code:

```
import numpy as np, pandas as pd
```

```python
# Times in minutes since 7:30
times_hr = ["7:30","7:45","8:00","8:15","8:45","9:15"]
times_min = np.array([0,15,30,45,75,105], dtype=float)  # minutes since 7:30
counts_per_4min = np.array([18,24,26,20,18,9], dtype=float) # Given counts per 4
↪  minutes at sample times
rate_per_min = counts_per_4min / 4.0 # Convert to rate per minute

df = pd.DataFrame({
    "Time": times_hr,
    "t_min_since_7_30": times_min,
    "counts_per_4min": counts_per_4min,
    "rate_per_minute": rate_per_min
})

# Composite trapezoidal with unequal spacing
total_cars = 0.0
terms = []
for i in range(len(times_min)-1):
    h = times_min[i+1] - times_min[i]  # minutes
    area = 0.5 * (rate_per_min[i] + rate_per_min[i+1]) * h
    total_cars += area
    terms.append((times_hr[i]+"-"+times_hr[i+1], h, rate_per_min[i], rate_per_min[i+1],
    ↪  area))

avg_rate_per_min = total_cars / (times_min[-1] - times_min[0])
pd.DataFrame(terms,
↪  columns=["Interval","Duration_min","rate_start","rate_end","cars_in_interval"])
```

Output:

Interval	Duration_min	rate_start	rate_end	cars_in_interval
7:30-7:45	15.0	4.5	6.00	78.75
7:45-8:00	15.0	6.0	6.50	93.75
8:00-8:15	15.0	6.5	5.00	86.25
8:15-8:45	0.0	5.0	4.50	142.50
8:45-9:15	30.0	4.5	2.25	101.25

5 Problem 5

Code:

```python
import math

def integrand(x):
    return math.exp(-x*x)

erf_exact = 0.966105

scale = math.sqrt(2.0 / math.pi)
scale_2 = 2.0 / math.sqrt(math.pi) # There seems to be a typo in the question, using
↪  the correct scale

def romberg_integration(a,b,levels):
    R = np.zeros((levels, levels))
    for k in range(levels):
        n = 2**k
```

```python
        h = (b - a) / n
        integral = 0.5 * (integrand(a) + integrand(b))
        for i in range(1, n):
            integral += integrand(a + i * h)
        integral *= h
        R[k,0] = integral
        for j in range(1, k+1):
            R[k,j] = R[k,j-1] + (R[k,j-1] - R[k-1,j-1]) / (4**j - 1)
    return R[levels-1, levels-1]

I_romberg = romberg_integration(0,1.5,4) * scale
print("Romberg Integration Approximation: ", I_romberg)
print("Exact Integral Value: ", erf_exact)
print("Relative Error: ", abs(erf_exact - I_romberg) / abs(erf_exact))
print()

def gauss_point_quadrature(a, b):
    points = [-1/math.sqrt(3), 1/math.sqrt(3)]
    weights = [1.0, 1.0]
    integral = 0.0
    for i in range(2):
        x_i = 0.5 * (b - a) * points[i] + 0.5 * (a + b)
        integral += weights[i] * integrand(x_i)
    integral *= 0.5 * (b - a)
    return integral

I_gauss2 = gauss_point_quadrature(0,1.5) * scale
print("2-Point Gauss Quadrature Approximation: ", I_gauss2)
print("Exact Integral Value: ", erf_exact)
print("Relative Error: ", abs(erf_exact - I_gauss2) / abs(erf_exact))
print()

I_romberg = romberg_integration(0,1.5,4) * scale_2
print("Romberg Integration Approximation: ", I_romberg)
print("Exact Integral Value: ", erf_exact)
print("Relative Error: ", abs(erf_exact - I_romberg) / abs(erf_exact))
print()

I_gauss2 = gauss_point_quadrature(0,1.5) * scale_2
print("2-Point Gauss Quadrature Approximation: ", I_gauss2)
print("Exact Integral Value: ", erf_exact)
print("Relative Error: ", abs(erf_exact - I_gauss2) / abs(erf_exact))
print()
```

Output:

```
Romberg Integration Approximation:  0.6831337632235525
Exact Integral Value:  0.966105
Relative Error:  0.29289905007887085

2-Point Gauss Quadrature Approximation:  0.6888444217517464
Exact Integral Value:  0.966105
Relative Error:  0.28698803778911564

Romberg Integration Approximation:  0.9660970328657184
Exact Integral Value:  0.966105
Relative Error:  8.246654640684995e-06

2-Point Gauss Quadrature Approximation:  0.974173123606372
Exact Integral Value:  0.966105
```

```
Relative Error:  0.00835118709288534
```

6 Problem 6

We start from the approximation

$$f'(x) \approx \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}.$$

To obtain the error series, expand each term about x by its Taylor series,

$$\begin{aligned}
f(x+h) &= f + hf' + \tfrac{h^2}{2}f'' + \tfrac{h^3}{6}f^{(3)} + \tfrac{h^4}{24}f^{(4)} + \tfrac{h^5}{120}f^{(5)} + \tfrac{h^6}{720}f^{(6)} + \tfrac{h^7}{5040}f^{(7)} + \cdots, \\
f(x-h) &= f - hf' + \tfrac{h^2}{2}f'' - \tfrac{h^3}{6}f^{(3)} + \tfrac{h^4}{24}f^{(4)} - \tfrac{h^5}{120}f^{(5)} + \tfrac{h^6}{720}f^{(6)} - \tfrac{h^7}{5040}f^{(7)} + \cdots, \\
f(x+2h) &= f + 2hf' + \tfrac{(2h)^2}{2}f'' + \tfrac{(2h)^3}{6}f^{(3)} + \tfrac{(2h)^4}{24}f^{(4)} + \tfrac{(2h)^5}{120}f^{(5)} + \tfrac{(2h)^6}{720}f^{(6)} + \tfrac{(2h)^7}{5040}f^{(7)} + \cdots, \\
f(x-2h) &= f - 2hf' + \tfrac{(2h)^2}{2}f'' - \tfrac{(2h)^3}{6}f^{(3)} + \tfrac{(2h)^4}{24}f^{(4)} - \tfrac{(2h)^5}{120}f^{(5)} + \tfrac{(2h)^6}{720}f^{(6)} - \tfrac{(2h)^7}{5040}f^{(7)} + \cdots.
\end{aligned}$$

The numerator,

$$N \;=\; f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h).$$

Substitute the expansions and collect terms by powers of h. Terms of even or odd orders cancel, hence,

$$N = 12\,h\,f' - \frac{2}{5}\,h^5 f^{(5)} - \frac{1}{21}\,h^7 f^{(7)} + \mathcal{O}(h^9)$$

Now divide by $12h$,

$$\frac{N}{12h} = f'(x) \;-\; \frac{1}{30}\,h^4 f^{(5)}(x) \;-\; \frac{1}{252}\,h^6 f^{(7)}(x) \;+\; \mathcal{O}(h^8).$$

Therefore the truncation error ε is,

$$\boxed{\varepsilon = -\frac{1}{30}\,h^4 f^{(5)}(x) \;-\; \frac{1}{252}\,h^6 f^{(7)}(x) \;-\; \frac{1}{9360}\,h^8 f^{(9)}(x) \;-\; \cdots}$$

and the leading term is

$$\boxed{\varepsilon = -\frac{1}{30}\,h^4\,f^{(5)}(x) + \mathcal{O}(h^6).}$$

Therefore,

$$\boxed{f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} - \frac{1}{30}\,h^4\,f^{(5)}(\xi),}$$

and hence the scheme is fourth-order accurate in h.

7 Problem 7

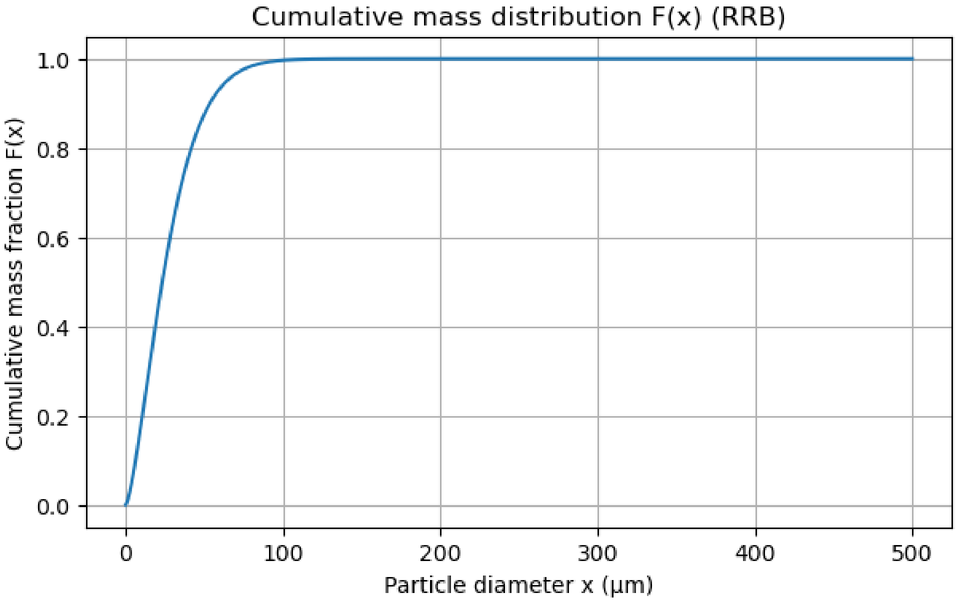
Code:

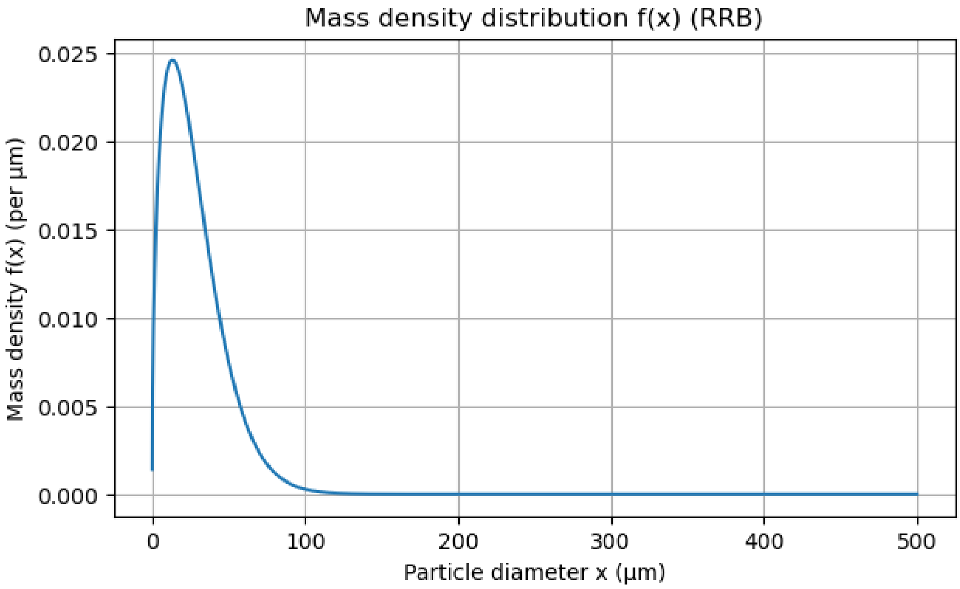
```
import numpy as np, math
import matplotlib.pyplot as plt

xprime_um = 30.0        # x' in micrometers
nprime = 1.44           # shape
```

```python
rho = 1.0                # g/cm^3
dmin_um = 1.0            # micrometers

def um_to_cm(x):
    return x * 1e-4
def cm_to_um(x):
    return x * 1e4
# Functions (x in micrometers)
def F_x(x):
    return 1.0 - np.exp(- (x / xprime_um)**nprime)
def f_x(x):
    # f(x) = n'/x' * (x/x')^{n'-1} * exp(-(x/x')^{n'})
    return (nprime / xprime_um) * (x / xprime_um)**(nprime - 1.0) * np.exp(- (x /
    ↪  xprime_um)**nprime)

# Mode x_mode = x' * ((n'-1)/n')^{1/n'}
if nprime > 1.0:
    x_mode_um = xprime_um * ((nprime - 1.0) / nprime)**(1.0 / nprime)
else:
    x_mode_um = None
x_vals = np.linspace(0.01, 500.0, 2000)  # micrometers from 0.01 to 500 um
F_vals = F_x(x_vals)
f_vals = f_x(x_vals)

dmin = dmin_um
x_max = 1e5 # micrometers
def composite_simpson(y, x):
    n = len(x) - 1
    if n % 2 == 1:
        x = x[:-1]; y = y[:-1]; n = len(x)-1
    h = (x[-1] - x[0]) / n
    S = y[0] + y[-1] + 4.0 * np.sum(y[1:-1:2]) + 2.0 * np.sum(y[2:-1:2])
    return S * h / 3.0

x_int = np.concatenate([np.linspace(dmin, 1000, 2000), np.logspace(np.log10(1000),
↪  np.log10(x_max), 2000)])
y_int = f_x(x_int) * (1e4 / x_int)  # Convert f(x) from per um to per cm
integral_val = composite_simpson(y_int, x_int)

Sm = (6.0 / rho) * integral_val # cm^2/g
print("Mass specific surface area Sm (cm^2/g): ", Sm)

# F(x)
plt.figure(figsize=(7,4))
plt.plot(x_vals, F_vals)
plt.title("Cumulative mass distribution F(x) (RRB)")
plt.xlabel("Particle diameter x (µm)")
plt.ylabel("Cumulative mass fraction F(x)")
plt.grid(True)
plt.show()

# f(x)
plt.figure(figsize=(7,4))
plt.plot(x_vals, f_vals)
plt.title("Mass density distribution f(x) (RRB)")
plt.xlabel("Particle diameter x (µm)")
plt.ylabel("Mass density f(x) (per µm)")
plt.grid(True)
plt.show()
```

Output:

```
Mass specific surface area Sm (cm^2/g):  220025.01208129118
```





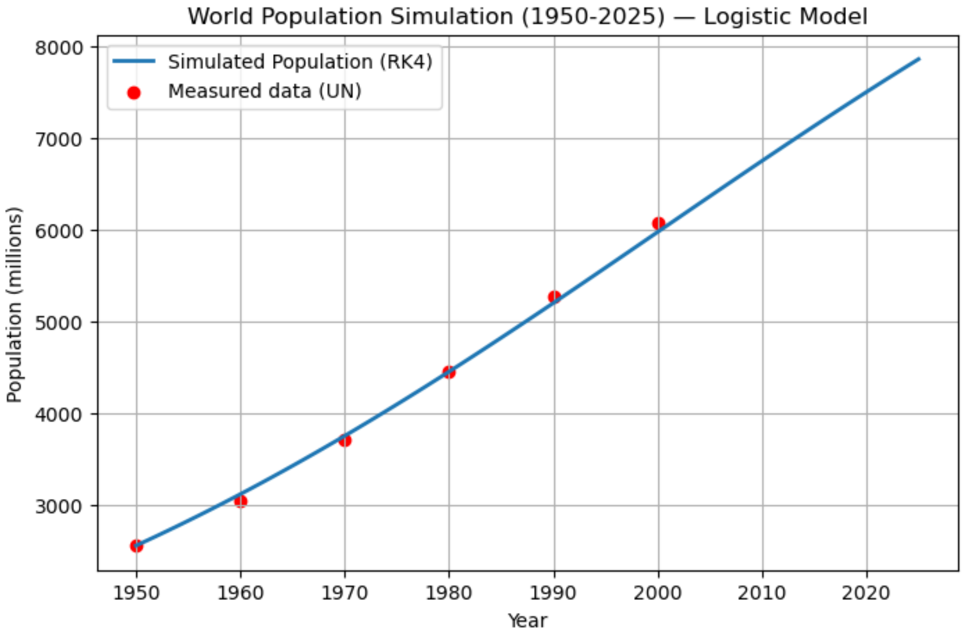
8 Problem 8

<u>Code:</u>

```
import numpy as np
import matplotlib.pyplot as plt

kgm = 0.026      # /yr
pmax = 12000.0   # million
p0 = 2555.0      # million in 1950
t0 = 1950
t_end = 2025

# Time step for numerical integration (1 yr resolution)
h = 1.0
```

```python
t_vals = np.arange(t0, t_end + h, h)

# ODE: dp/dt = kgm * (1 - p/pmax) * p
def dpdt(p):
    return kgm * (1.0 - p / pmax) * p

# RK4
p_vals = [p0]
for i in range(1, len(t_vals)):
    p = p_vals[-1]
    k1 = dpdt(p)
    k2 = dpdt(p + 0.5*h*k1)
    k3 = dpdt(p + 0.5*h*k2)
    k4 = dpdt(p + h*k3)
    p_next = p + (h/6.0)*(k1 + 2*k2 + 2*k3 + k4)
    p_vals.append(p_next)

p_vals = np.array(p_vals)

# UN Data
data_years = np.array([1950, 1960, 1970, 1980, 1990, 2000])
data_pop = np.array([2555, 3040, 3708, 4454, 5276, 6079])

# Simulation prediction for 2025
p_2025_pred = p_vals[-1]

# Plot
plt.figure(figsize=(8,5))
plt.plot(t_vals, p_vals, label='Simulated Population (RK4)', lw=2)
plt.scatter(data_years, data_pop, color='red', label='Measured data (UN)')
plt.title("World Population Simulation (1950-2025) — Logistic Model")
plt.xlabel("Year")
plt.ylabel("Population (millions)")
plt.legend()
plt.grid(True)
plt.show()
```

Output:



9 Problem 9

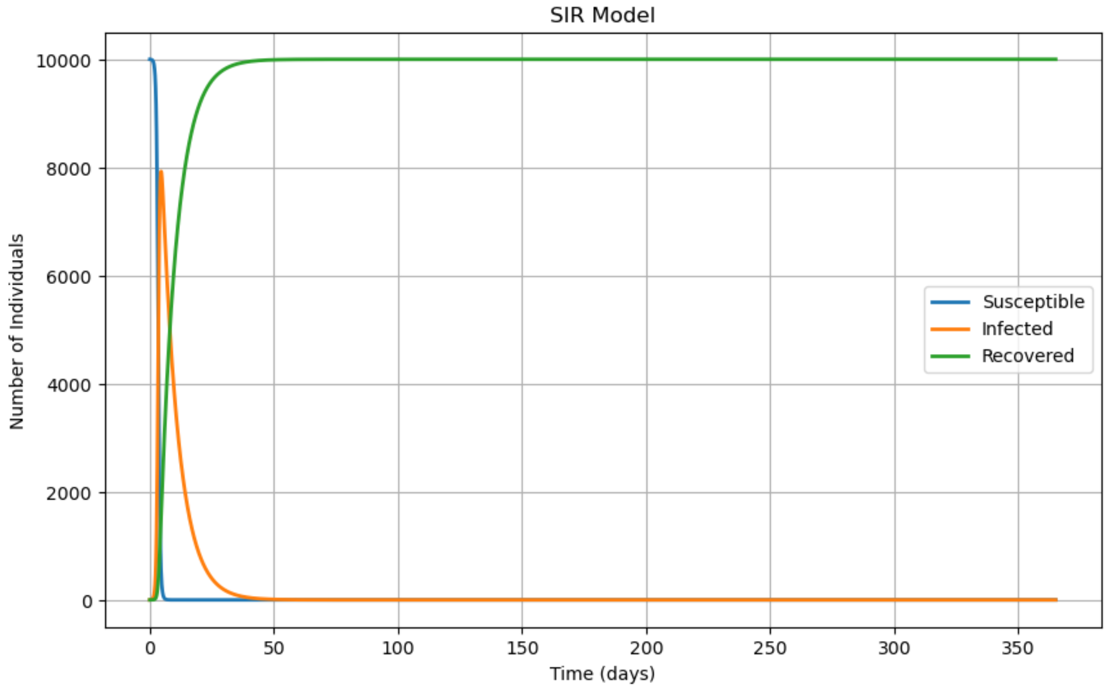
Code:

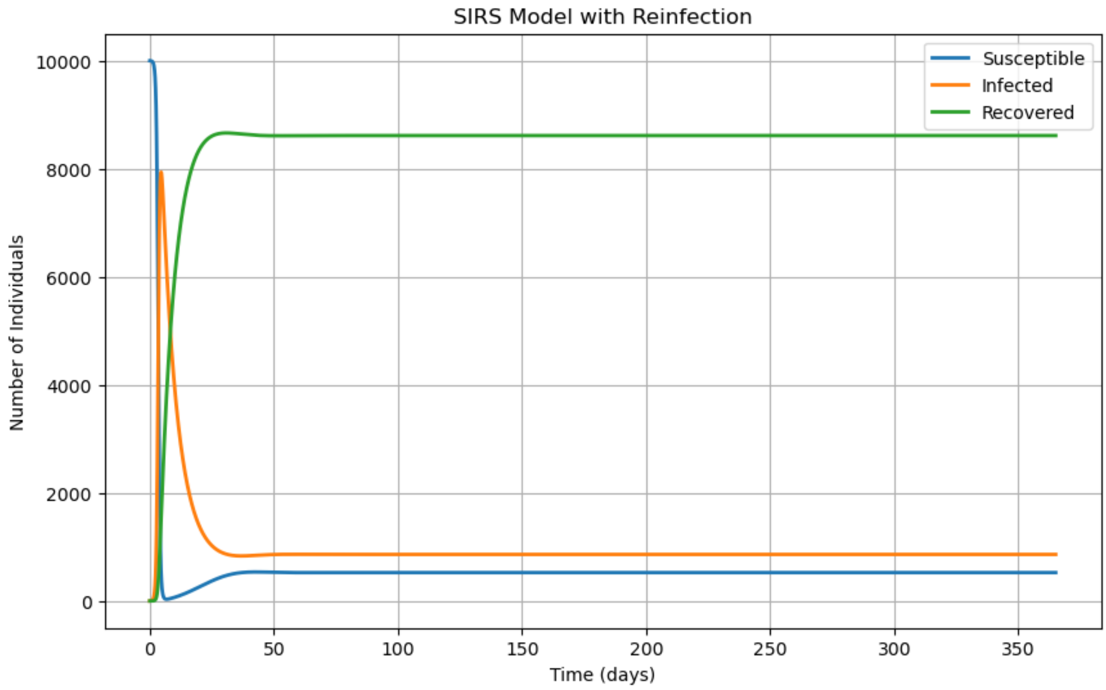
```python
import numpy as np, math, matplotlib.pyplot as plt

# Initial Conditions
N = 10000.0            # total population
S0 = 9999.0
I0 = 1.0
R0 = 0.0

# Rates
a_per_week = 0.002                      # per person per week
a = a_per_week / 7.0                    # per person per day
r = 0.15                                # per day recovery rate

def simulate_sir(a, r, S0, I0, R0, t_max=365.0, dt=0.1):
    t = np.arange(0.0, t_max+dt, dt)
    S = np.zeros_like(t)
    I = np.zeros_like(t)
    R = np.zeros_like(t)
    S[0], I[0], R[0] = S0, I0, R0
    for n in range(len(t)-1):
        # RK4 step
        p = lambda S,I,R: np.array([ -a*S*I, a*S*I - r*I, r*I ])
        y = np.array([S[n], I[n], R[n]])
        k1 = p(*y)
        k2 = p(*(y + 0.5*dt*k1))
        k3 = p(*(y + 0.5*dt*k2))
        k4 = p(*(y + dt*k3))
        y_next = y + (dt/6.0)*(k1 + 2*k2 + 2*k3 + k4)
        y_next = np.maximum(y_next, 0.0) # ensure non-negativity and conservation
        S[n+1], I[n+1], R[n+1] = y_next
    return t, S, I, R

t_a, S_a, I_a, R_a = simulate_sir(a, r, S0, I0, R0, t_max=365.0, dt=0.1)

# time when infected falls below 10 after epidemic has started (I>1)
idx_after_peak = np.where(I_a < 10.0)[0]
t_below_10 = None
if len(idx_after_peak)>0: # choose first time index where I<10 and time>0
    for idx in idx_after_peak:
        if t_a[idx] > 0.0:
            t_below_10 = t_a[idx]
            break

print("Time when infected falls below 10: ", t_below_10, " days")

peak_I = I_a.max()
t_peak = t_a[I_a.argmax()]

rho = 0.015  # per day
def simulate_sirs_reinfection(a, r, rho, S0, I0, R0, t_max=365.0, dt=0.1):
    t = np.arange(0.0, t_max+dt, dt)
    S = np.zeros_like(t)
    I = np.zeros_like(t)
    R = np.zeros_like(t)
    S[0], I[0], R[0] = S0, I0, R0
    for n in range(len(t)-1):
        def p_val(S,I,R):
```

```
            return np.array([ -a*S*I + rho*R, a*S*I - r*I, r*I - rho*R ])
        y = np.array([S[n], I[n], R[n]])
        k1 = p_val(*y)
        k2 = p_val(*(y + 0.5*dt*k1))
        k3 = p_val(*(y + 0.5*dt*k2))
        k4 = p_val(*(y + dt*k3))
        y_next = y + (dt/6.0)*(k1 + 2*k2 + 2*k3 + k4)
        y_next = np.maximum(y_next, 0.0)
        S[n+1], I[n+1], R[n+1] = y_next
    return t, S, I, R

t_b, S_b, I_b, R_b = simulate_sirs_reinfection(a, r, rho, S0, I0, R0, t_max=365.0,
 ↪  dt=0.1)

idx_after_peak_b = np.where(I_b < 10.0)[0]
t_below_10_b = None
if len(idx_after_peak_b)>0:
    for idx in idx_after_peak_b:
        if t_b[idx] > 0.0:
            t_below_10_b = t_b[idx]
            break

print("Time when infected falls below 10 (with reinfection): ", t_below_10_b, " days")

peak_I_b = I_b.max()
t_peak_b = t_b[I_b.argmax()]

plt.figure(figsize=(10,6))
plt.plot(t_a, S_a, label='Susceptible', lw=2)
plt.plot(t_a, I_a, label='Infected', lw=2)
plt.plot(t_a, R_a, label='Recovered', lw=2)
plt.title("SIR Model")
plt.xlabel("Time (days)")
plt.ylabel("Number of Individuals")
plt.legend()
plt.grid(True)
plt.show()

plt.figure(figsize=(10,6))
plt.plot(t_b, S_b, label='Susceptible', lw=2)
plt.plot(t_b, I_b, label='Infected', lw=2)
plt.plot(t_b, R_b, label='Recovered', lw=2)
plt.title("SIRS Model with Reinfection")
plt.xlabel("Time (days)")
plt.ylabel("Number of Individuals")
plt.legend()
plt.grid(True)
plt.show()
```

Output:

```
Time when infected falls below 10:  0.1  days
Time when infected falls below 10 (with reinfection):  0.1  days
```


SIR Model
Number of Individuals
Time (days)
Susceptible
Infected
Recovered
0
2000
4000
6000
8000
10000
0
50
100
150
200
250
300
350


SIRS Model with Reinfection
Number of Individuals
Time (days)
Susceptible
Infected
Recovered
0
2000
4000
6000
8000
10000
0
50
100
150
200
250
300
350