

HT 2019

PROBLEM SHEET 2

Optimization, Convexity, Lagrange Multipliers, and Numerical Integration

2.1. We want to find and classify the stationary points of :

$$(a) \ g(x, y) = e^{x^3-3x} e^{y^3-3y}$$

$$\frac{dg}{dx} = 0 \Leftrightarrow \frac{\partial g}{\partial x} = 0 \text{ and } \frac{\partial g}{\partial y} = 0$$

$$\frac{\partial g}{\partial x} = 0 \Leftrightarrow \underbrace{e^{x^3-3x}}_{\neq 0} (3x^2-3) \underbrace{e^{y^3-3y}}_{\neq 0} = 0 \Leftrightarrow 3(x^2-1) = 0 \Leftrightarrow x = \pm 1$$

$$\frac{\partial g}{\partial y} = 0 \Leftrightarrow \underbrace{e^{x^3-3x}}_{\neq 0} \underbrace{e^{y^3-3y}}_{\neq 0} (3y^2-3) = 0 \Leftrightarrow 3(y^2-1) = 0 \Leftrightarrow y = \pm 1$$

We have the following stationary points for g : $(-1, -1)$, $(-1, 1)$, $(1, -1)$ and $(1, 1)$.

To classify them, we need the Hessian of g

$$\frac{\partial^2 g}{\partial x^2} = e^{y^3-3y} \left(e^{x^3-3x} (3x^2-3)^2 + e^{x^3-3x} (6x) \right)$$

$$\frac{\partial^2 g}{\partial x \partial y} = \frac{\partial^2 g}{\partial y \partial x} = e^{x^3-3x} (3x^2-3) e^{y^3-3y} (3y^2-3)$$

$$\frac{\partial^2 g}{\partial y^2} = e^{x^3-3x} \left(e^{y^3-3y} (3y^2-3)^2 + e^{y^3-3y} (6y) \right)$$

Then, we have:

$$H(g)(-1, -1) = \begin{pmatrix} -6e^4 & 0 \\ 0 & -6e^4 \end{pmatrix} = -6e^4 I, \text{ which is negative definite} \Rightarrow (-1, -1) \text{ is a LOCAL MAXIMUM for } g$$

$$H(g)(-1, 1) = \begin{pmatrix} -6 & 0 \\ 0 & 6 \end{pmatrix}, \text{ which is indefinite as } \begin{vmatrix} -6 & 0 \\ 0 & 6 \end{vmatrix} = -36 < 0 \Rightarrow (-1, 1) \text{ is a SADDLE POINT for } g$$

$$H(g)(1, -1) = \begin{pmatrix} 6 & 0 \\ 0 & -6 \end{pmatrix}, \text{ which is indefinite as } \begin{vmatrix} 6 & 0 \\ 0 & -6 \end{vmatrix} = -36 < 0 \Rightarrow (1, -1) \text{ is a SADDLE POINT for } g$$

$$H(g)(1, 1) = \begin{pmatrix} 6e^{-4} & 0 \\ 0 & 6e^{-4} \end{pmatrix} = 6e^{-4} I, \text{ which is positive definite} \Rightarrow (1, 1) \text{ is a LOCAL MINIMUM for } g$$

$$(b) h(x, y, z) = \frac{1}{2} x^2 + y^2 + \frac{27}{2} z^2 - xy + xz + 4yz - x - y - 11z$$

$$\frac{\partial h}{\partial x} = x - y + z - 1$$

$$\frac{\partial h}{\partial y} = -x + 2y + 4z - 1$$

$$\frac{\partial h}{\partial z} = x + 4y + 27z - 11$$

$$\frac{dh}{dx} = 0$$

$$\Rightarrow \begin{cases} x - y + z - 1 = 0 \Rightarrow x = y - z + 1 \\ -x + 2y + 4z - 1 = 0 \\ x + 4y + 27z - 11 = 0 \end{cases} \Rightarrow \begin{cases} y + 3z = 2 \\ 5y - 26z = 10 \end{cases} \Rightarrow y = 2, z = 0 \Rightarrow x = 3$$

So, the only stationary point that h has is $(3, 2, 0)$.

Let's find the Hessian:

$$\frac{\partial^2 h}{\partial x^2} = 1; \quad \frac{\partial^2 h}{\partial y^2} = 2; \quad \frac{\partial^2 h}{\partial z^2} = 27; \quad \frac{\partial^2 h}{\partial x \partial y} = -1; \quad \frac{\partial^2 h}{\partial x \partial z} = 1; \quad \frac{\partial^2 h}{\partial y \partial z} = 4$$

$$\text{So, } H(h)(3, 2, 0) = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 2 & 4 \\ 1 & 4 & 27 \end{pmatrix}$$

We have the upper-left submatrix $\begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}$ with eigenvalues $\lambda_1 = \frac{3-\sqrt{5}}{2} > 0$, $\lambda_2 = \frac{3+\sqrt{5}}{2} > 0 \Rightarrow$ it is positive definite $\Rightarrow H(h)(3, 2, 0)$ is positive definite $\Rightarrow (3, 2, 0)$ is a local minimum.

2.2. Let $\underline{a} \in \mathbb{R}^n$ with $a_i > 0$ and $\sum_i a_i = 1$

Let $\Delta_a =$ diagonal matrix with \underline{a} on the diagonal

We have $\Delta_a - \underline{a}\underline{a}^T$ positive semidefinite if $\underline{a}^T \Delta_a^{-1} \underline{a} \leq 1$.

$$\Delta_a = \begin{pmatrix} a_1 & 0 & 0 & \dots & 0 \\ 0 & a_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & a_n \end{pmatrix} \Rightarrow \Delta_a^{-1} = \begin{pmatrix} \frac{1}{a_1} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{a_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{a_n} \end{pmatrix}$$

$$\underline{a}^T \Delta_a^{-1} \underline{a} = (a_1, a_2, \dots, a_n) \begin{pmatrix} \frac{1}{a_1} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{a_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{a_n} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \underline{1} \cdot \underline{a} = \sum_i a_i = 1 \leq 1 \Rightarrow$$

$\Rightarrow \Delta_a - \underline{a}\underline{a}^T$ is positive semidefinite.

We want to prove that l is convex, where

$$l(\underline{x}) = \ln \left(\sum_{i=1}^n e^{x_i} \right)$$

$l = f \circ g$, where $f: \mathbb{R} \rightarrow \mathbb{R}$, $f(x) = \ln x$, which is concave and strictly increasing
 $g: \mathbb{R}^n \rightarrow \mathbb{R}$, $g(\underline{x}) = \sum_{i=1}^n e^{x_i}$, which is convex, as a sum of convex functions \Rightarrow

$\Rightarrow f \circ g$ is convex, therefore l is convex.

Alternative solution

$$\frac{dl}{d\underline{x}} = \frac{1}{\sum_{i=1}^n e^{x_i}} \cdot \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix}$$

$$H(l) = J \left(\frac{dl}{d\underline{x}} \right) = J \left(\frac{1}{\sum_{i=1}^n e^{x_i}} \cdot \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix} \right) = \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix} \cdot \left(- \frac{1}{\left(\sum_{i=1}^n e^{x_i} \right)^2} \cdot \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix}^T \right) +$$

$$+ \frac{1}{\sum_{i=1}^n e^{x_i}} \cdot \begin{pmatrix} e^{x_1} & 0 & 0 & \dots & 0 \\ 0 & e^{x_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & e^{x_n} \end{pmatrix} = - \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix} \cdot (e^{x_1} \ e^{x_2} \ \dots \ e^{x_n}) \cdot \frac{1}{\left(\sum_{i=1}^n e^{x_i} \right)^2} + \frac{1}{\sum_{i=1}^n e^{x_i}}$$

$$= \begin{pmatrix} e^{x_1} & 0 & 0 & \dots & 0 \\ 0 & e^{x_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & e^{x_n} \end{pmatrix}$$

$$\text{Let } \underline{a} = \frac{1}{\sum_{i=1}^n e^{x_i}} \cdot \begin{pmatrix} e^{x_1} \\ e^{x_2} \\ \vdots \\ e^{x_n} \end{pmatrix} \Rightarrow a_i > 0 \text{ and } \sum_{i=1}^n a_i = 1 \text{ and}$$

$H(l) = -\underline{a} \cdot \underline{a}^T + \Delta_a$, which we know it's positive semi-definite, therefore l is convex.

2.3. X, Y, Z with costs p, q, r respectively, $p, q, r > 0$ different, budget $B > 0$.

The value of a product is $g(x, y, z)$.

(a) We want to maximise f on

$$F = \left\{ (x, y, z) \mid x, y, z \geq 0, \ p x + q y + r z - B \leq 0 \right\}$$

(b) $g(x, y, z) = x y z$

We have g increasing in all dimensions, so if we want to maximize g with the constraint $p x + q y + r z - B \leq 0$, we need to have equality there, so the constraint has to be tight, therefore we can transform it into an equality constraint.

$$\text{Let } \Lambda(1, \underline{v}) = xyz + (B - px - qy - rz)\lambda, \quad \underline{v} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

We need

$$B - px - qy - rz = 0$$

$$\begin{cases} yz = p\lambda \\ xz = q\lambda \\ xy = r\lambda \end{cases} \Rightarrow \begin{cases} x = \sqrt{\frac{1qn}{p}} \\ y = \sqrt{\frac{1pn}{q}} \\ z = \sqrt{\frac{1pq}{n}} \end{cases} \Rightarrow B = 3\sqrt{1pqn} \Rightarrow \lambda = \frac{B^2}{9pqn} \Rightarrow$$

$$\Rightarrow x = \frac{B}{3p}, y = \frac{B}{3q}, z = \frac{B}{3n} \text{ (all positive)} \Rightarrow \text{the maximum of } g \text{ on } F \text{ is } \frac{B^3}{27pqn}.$$

(c) We now want to maximise $g(\underline{v}) = e^{x+y+z}$, which is also increasing in every dimension, on F . So, we need: $\Lambda(1, \underline{v}) = e^{x+y+z} + (B - px - qy - rz)\lambda$

$$B - px - qy - rz = 0$$

$$\begin{cases} e^{x+y+z} = \lambda p \\ e^{x+y+z} = \lambda q \\ e^{x+y+z} = \lambda n \end{cases} \Rightarrow \lambda = 0 \Rightarrow e^{x+y+z} = 0, \text{ which is impossible!}$$

Notice that we didn't succeed with set of constraints we have, so we need to try all the possibilities of combinations of tight/slack constraints. We keep $B - px - qy - rz = 0$, as that is obvious from the increasing nature of g in all dimensions. For $x=0$ and $y, z \neq 0$ we get

$$\begin{cases} e^{y+z} = \lambda q \\ e^{y+z} = \lambda n \end{cases} \Rightarrow \lambda = 0 \Rightarrow e^{y+z} = 0, \text{ which is impossible!}$$

For $x=y=0$, we get

$$g(x, y, z) = g(0, 0, z) = e^z$$

$$\Lambda(1, \underline{v}) = e^z + (B - rz)\lambda$$

$$\Lambda(1, \underline{v}) = e^z + B\lambda - rz\lambda$$

$$B - rz = 0 \Rightarrow z = \frac{B}{n}$$

$$e^z = r\lambda \Rightarrow \lambda = \frac{e^z}{n} = \frac{e^{\frac{B}{n}}}{n} \Rightarrow e^{\frac{B}{n}} \text{ is the maximum}$$

To get the maximum value, we need $\max\left\{\frac{B}{p}, \frac{B}{q}, \frac{B}{n}\right\}$, which is $\frac{B}{\min\{p, q, n\}} := \min \Rightarrow$

\Rightarrow the result is $e^{\frac{B}{\min\{p, q, n\}}}$.

2.4. $w_{ij} = w_{ji}$

minimize $E(\underline{x}) = \sum_i \sum_j w_{ij} (x_i - x_j)^2$ subject to $\sum_i x_i^2 = 1, \sum_i x_i = 0.$

(a)
$$E(\underline{x}) = \sum_i \sum_j w_{ij} (x_i - x_j)^2 = \sum_i \sum_j w_{ij} (x_i^2 - 2x_i x_j + x_j^2) =$$

$$= 2 \sum_i \sum_j w_{ij} x_i^2 - 2 \sum_i \sum_j x_i x_j w_{ij} =$$

$$\sum_i \sum_j w_{ij} x_i^2 = \sum_i x_i^2 \sum_j w_{ij} = \sum_i x_i^2 \sum_j w_{ji} = \underline{x}^T \underline{D} \underline{x},$$
 where \underline{D} is the diagonal matrix that satisfies $\underline{1}^T \underline{D} = \underline{1}^T \underline{W}$, and \underline{W} is the symmetric matrix (w_{ij})

$$\sum_i \sum_j x_i x_j w_{ij} = \underline{x}^T \underline{W} \underline{x}$$

So, $E(\underline{x}) = 2 \underline{x}^T \underline{D} \underline{x} - 2 \underline{x}^T \underline{W} \underline{x} = 2 \underline{x}^T (\underline{D} - \underline{W}) \underline{x}$

We have $\sum_i x_i^2 = 1 \Rightarrow \underline{x}^T \underline{x} = 1$ and $\sum_i x_i = 0 \Rightarrow \underline{1}^T \underline{x} = 0$

(b) We have $\underline{x}^T (\underline{D} - \underline{W}) \underline{x} = \frac{1}{2} \sum_i \sum_j \underbrace{w_{ij}}_{\geq 0} \underbrace{(x_i - x_j)^2}_{\geq 0} \geq 0 \quad (\forall) \underline{x} \in \mathbb{R}^n \Rightarrow$

$\Rightarrow (\underline{D} - \underline{W})$ is positive semidefinite

(c) $\frac{dE}{d\underline{x}} = 2 \cdot 2 (\underline{D} - \underline{W}) \cdot \underline{x} = 4 (\underline{D} - \underline{W}) \underline{x}$

$\frac{d}{d\underline{x}} \left(\sum_i x_i^2 \right) = 2 \underline{x}$

$\frac{d}{d\underline{x}} \left(\sum_i x_i \right) = \underline{1}$

\Rightarrow The first-order condition for a stationary point of the Lagrangian is

$4(\underline{D} - \underline{W}) \underline{x} - 2\lambda \underline{x} - \mu \underline{1} = \underline{0} \quad (*)$

By multiplying $(*)$ with $\underline{1}^T$, we get:

$$\underbrace{4 \underline{1}^T (\underline{D} - \underline{W}) \underline{x}}_{=0} - \underbrace{2\lambda \underline{1}^T \underline{x}}_{=0} - \mu \underline{1}^T \underline{1} = 0 \Rightarrow \mu n = 0 \quad (\forall) n \in \mathbb{N}^* \Rightarrow \mu = 0$$

(d) Let $\underline{x} \in \mathbb{R}^n$ be a solution to $(*)$. Then:

$4(\underline{D} - \underline{W}) \underline{x} = 2\lambda \underline{x}$

$(\underline{D} - \underline{W}) \underline{x} = \frac{1}{2} \lambda \underline{x}$, where $\frac{1}{2} \lambda \in \mathbb{R} \Rightarrow \underline{x}$ is an eigenvector of $(\underline{D} - \underline{W})$ with the corresponding eigenvalue $\frac{1}{2} \lambda = \lambda$

Then, we have

as long as the constraints are satisfied

$$E(\underline{x}) = 2 \underline{x}^T (\Delta - W) \underline{x} = 2 \underline{x}^T \lambda \underline{x} = 2 \lambda \underline{x}^T \underline{x} = 2 \lambda$$

$$(\Delta - W) \underline{x} = \begin{pmatrix} \sum_{j=1}^n w_{j1} - w_{11} & -w_{12} & \dots & -w_{1n} \\ -w_{21} & \sum_{j=1}^n w_{j2} - w_{22} & \dots & -w_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -w_{n1} & -w_{n2} & \dots & \sum_{j=1}^n w_{jn} - w_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} \lambda x_1 \\ \lambda x_2 \\ \vdots \\ \lambda x_n \end{pmatrix}$$

Let c_j be the sum on the j th column of $\Delta - W$. Then $c_j = 0 \ (\forall) j \in \{1, 2, \dots, n\}$

Then the vector from LHS has the sum of the elements 0 (because it is $\sum_j c_j x_j$), so

$$\mathbf{1}^T (\Delta - W) \underline{x} = 0 \Rightarrow \mathbf{1}^T \lambda \underline{x} = 0 \Rightarrow \lambda (\mathbf{1}^T \underline{x}) = 0$$

if $\lambda = 0$, then \underline{x} can be any vector, so it doesn't necessarily have $\mathbf{1}^T \underline{x} = 0$.

Unless $\lambda = 0$, we have $\mathbf{1}^T \underline{x} = 0$.

(e) Let \underline{x} be the solution to the optimization problem. Then we have

$$\sum_i x_i^2 = 1 \Rightarrow \underline{x}^T \underline{x} = 1 \Rightarrow \underline{x} \text{ is a unit vector}$$

From (d), we know that \underline{x} is an eigenvector of $(\Delta - W)$ and its eigenvalue λ is non-zero.

As $\Delta - W$ is positive semi-definite, $\lambda > 0$.

We have that $\frac{dE}{d\underline{x}} = 4(\Delta - W)\underline{x}$ and $H(E) = 4(\Delta - W)$, which is positive semi-definite, so E is a convex function. Then, if \underline{x} is a local minimum for E , then it must also be a global minimum.

We know that all the solutions are eigenvectors of $(\Delta - W)$ with non-zero eigenvalues. We will prove that if λ is the smallest eigenvalue of $(\Delta - W)$ (non-zero), then it is the minimum of E :

Let's suppose that $(\exists) \underline{v} \in \mathbb{R}^n$ eigenvector of $(\Delta - W)$ with corresponding eigenvalue $\alpha \geq \lambda$. Then, we have

$$\begin{aligned} E(\underline{x}) &= 2 \underline{x}^T (\Delta - W) \underline{x} = 2 \underline{x}^T \lambda \underline{x} = 2 \lambda \underline{x}^T \underline{x} = 2 \lambda \\ E(\underline{v}) &= 2 \underline{v}^T (\Delta - W) \underline{v} = 2 \underline{v}^T \alpha \underline{v} = 2 \alpha \underline{v}^T \underline{v} = 2 \alpha \geq 2 \lambda \end{aligned} \quad \Bigg| \Rightarrow E(\underline{x}) \leq E(\underline{v}) \Rightarrow \underline{x} \text{ is the global minimum of } E, \text{ so it is the solution of the optimization problem. (As } \lambda \text{ is the smallest eigenvalue which is non-zero, and because the smallest eigenvalue of } (\Delta - W) \text{ is } 0, \text{ then } \lambda \text{ is the second-smallest eigenvalue of } (\Delta - W)).$$

2.5. Let $f(x) = e^{e^x}$. We will compute the first 4 derivatives of f : (all of them increasing strictly)

$$\frac{df}{dx} = e^{e^x} \cdot e^x$$

$$\frac{d^2f}{dx^2} = e^{e^x} \cdot e^{2x} + e^{e^x} \cdot e^x = e^{e^x+2x} + e^{e^x+x}$$

$$\frac{d^3f}{dx^3} = e^{e^x+2x} \cdot (e^x+2) + e^{e^x+x} \cdot (e^x+1) = e^{e^x+3x} + 3e^{e^x+2x} + e^{e^x+x}$$

$$\frac{d^4f}{dx^4} = e^{e^x+3x} \cdot (e^x+3) + 3e^{e^x+2x} \cdot (e^x+2) + e^{e^x+x} \cdot (e^x+1) = e^{e^x+4x} + 6e^{e^x+3x} + 7e^{e^x+2x} + e^{e^x+x}$$

(a) Using the Midpoint rule: (to calculate $\int_0^1 f(x) dx$ with n strips)

$$-\frac{1}{24n^2} \bar{D}_2 \leq \text{err}(M_n)[f, 0, 1] \leq \frac{1}{24n^2} \underline{D}_2$$

$$\bar{D}_2 = \max_{x \in (0,1)} \frac{d^2f}{dx^2} = \frac{d^2f}{dx^2}(1) = e^{e+2} + e^{e+1} \approx 153.17$$

$$\underline{D}_2 = \min_{x \in (0,1)} \frac{d^2f}{dx^2} = \frac{d^2f}{dx^2}(0) = e^1 + e^1 = 2e \approx 5.44$$

We want $|\text{err}(M_n)[f, 0, 1]| < 10^{-6}$, but $|\text{err}(M_n)[f, 0, 1]| \leq \frac{1}{24n^2} \bar{D}_2$, so we want n such that

$$\frac{1}{24n^2} \cdot 153.17 \leq 10^{-6}$$

$$6.38 \cdot 10^6 \leq n^2$$

$$2.526 \cdot 10^3 \leq n \Rightarrow \boxed{n \geq 2526}$$

(b) Using the Trapezium rule:

$$\frac{1}{12n^2} \underline{D}_2 \leq \text{err}(T_n)[f, a, b] \leq \frac{1}{12n^2} \bar{D}_2$$

$$\frac{1}{12n^2} \cdot 153.17 \leq 10^{-6}$$

$$12.764 \cdot 10^6 \leq n^2$$

$$3.573 \cdot 10^3 \leq n \Rightarrow \boxed{n \geq 3573}$$

(c) Using Simpson's rule:

$$\frac{1}{180n^4} \underline{D}_4 \leq \text{err}(S_n)[f, 0, 1] \leq \frac{1}{180n^4} \bar{D}_4$$

$$\underline{D}_4 = \min_{x \in (0,1)} \frac{d^4f}{dx^4} = e^1 + 6e^1 + 7e^1 + e^1 = 15e \approx 40.77$$

$$\overline{\Delta}_4 = \max_{x \in (0,1)} \frac{d^4 f}{dx^4} = e^{e+4} + 6e^{e+3} + 7e^{e+2} + e^{e+1} \approx 3478.71$$

$$\frac{1}{180 n^4} \cdot 3478.71 \leq 10^{-6}$$

$$19.326 \cdot 10^6 \leq n^4 \Rightarrow \boxed{n \geq 67}$$

$$\boxed{2.6.} \quad \hat{f}_3(x) = f(l) + (x-l) \frac{df}{dx}(l) + \frac{(x-l)^2}{2} \frac{d^2 f}{dx^2}(l) + \frac{(x-l)^3}{6} \frac{d^3 f}{dx^3}(l)$$

$$(a) \quad A_1[f, 0, 2l] = \int_0^{2l} \hat{f}_3(x) dx = \int_0^{2l} \left[f(l) + (x-l) \frac{df}{dx}(l) + \frac{(x-l)^2}{2} \frac{d^2 f}{dx^2}(l) + \frac{(x-l)^3}{6} \frac{d^3 f}{dx^3}(l) \right] dx$$

$$A_1[f, 0, 2l] = \left[x f(l) + \frac{(x-l)^2}{2} \frac{df}{dx}(l) + \frac{(x-l)^3}{6} \frac{d^2 f}{dx^2}(l) + \frac{(x-l)^4}{24} \frac{d^3 f}{dx^3}(l) \right]_0^{2l}$$

$$A_1[f, 0, 2l] = 2l f(l) + \frac{2l^3}{6} \frac{d^2 f}{dx^2}(l) = 2l f(l) + \frac{l^3}{3} \frac{d^2 f}{dx^2}(l)$$

$$(b) \quad \underline{\Delta}_4 = \min_{\xi \in (0, 2l)} \left| \frac{d^4 f}{dx^4}(\xi) \right|, \quad \overline{\Delta}_4 = \max_{\xi \in (0, 2l)} \left| \frac{d^4 f}{dx^4}(\xi) \right|$$

$$f(x) = \hat{f}_3(x) + \frac{(x-l)^4}{24} \frac{d^4 f}{dx^4}(\xi), \text{ with } \xi \in (0, 2l)$$

$$\hat{f}_3(x) - f(x) = - \frac{(x-l)^4}{24} \cdot \frac{d^4 f}{dx^4}(\xi)$$

$$\underline{\Delta}_4 \leq \frac{d^4 f}{dx^4}(\xi) \leq \overline{\Delta}_4 \quad | \cdot \left(-\frac{(x-l)^4}{24} \right) \leq 0$$

$$- \frac{(x-l)^4}{24} \overline{\Delta}_4 \leq \hat{f}_3(x) - f(x) \leq - \frac{(x-l)^4}{24} \underline{\Delta}_4$$

(c) We have that (from (b))

$$\frac{(x-l)^4}{24} \underline{\Delta}_4 \leq f(x) - \hat{f}_3(x) \leq \frac{(x-l)^4}{24} \overline{\Delta}_4$$

$$\int_0^{2l} \frac{(x-l)^4}{24} \underline{\Delta}_4 dx \leq \int_0^{2l} f(x) dx - \int_0^{2l} \hat{f}_3(x) dx \leq \int_0^{2l} \frac{(x-l)^4}{24} \overline{\Delta}_4 dx$$

$$\frac{l^5}{60} \underline{\Delta}_4 \leq \int_0^{2l} f(x) dx - A_1[f, 0, 2l] \leq \frac{l^5}{60} \overline{\Delta}_4 \quad | \cdot (-1)$$

$$- \frac{1}{60} l^5 \overline{\Delta}_4 \leq \text{err}(A_1)[f, 0, 2l] \leq - \frac{1}{60} l^5 \underline{\Delta}_4$$

(d) From the subtasks above, we have

$$A_1[f, 0, 2l] = 2lf(l) + \frac{l^3}{3} \frac{d^2 f}{dx^2}(l)$$

$$-\frac{1}{60} l^5 \overline{\Delta}_4 \leq \text{err}(A_1)[f, 0, 2l] \leq -\frac{1}{60} l^5 \underline{\Delta}_4$$

First, we express a single strip from c to d

$$\begin{aligned} A_1[f, c, d] &= \frac{d-c}{2l} A_1\left[x \mapsto f\left(c + \frac{d-c}{2l}x\right), 0, 2l\right] = \\ &= \frac{d-c}{2l} \left(2l f\left(c + \frac{d-c}{2l}l\right) + \frac{l^3}{3} \frac{d^2 f}{dx^2}\left(c + \frac{d-c}{2l}l\right) \right) = \\ &= (d-c) f\left(\frac{c+d}{2}\right) + \frac{d-c}{2l} \cdot \frac{l^3}{3} \cdot \frac{(d-c)^2}{4l^2} \cdot \frac{d^2 f}{dx^2}\left(\frac{c+d}{2}\right) \\ &= (d-c) f\left(\frac{c+d}{2}\right) + \frac{(d-c)^3}{24} \cdot \frac{d^2 f}{dx^2}\left(\frac{c+d}{2}\right) \quad (*) \end{aligned}$$

$$\begin{aligned} \text{err}(A_1)[f, c, d] &= \frac{d-c}{2l} \text{err}(A_1)\left[x \mapsto f\left(c + \frac{d-c}{2l}x\right), 0, 2l\right] \leq \\ &\leq \left(\frac{d-c}{2l}\right) \left(-\frac{1}{60} l^5 \min_{x \in (0, 2l)} \frac{d^4 f}{dx^4}\left(c + \frac{d-c}{2l}x\right)\right) = \\ &= \frac{d-c}{2l} \cdot \left(-\frac{1}{60} l^5\right) \cdot \min_{x \in (c, d)} \frac{d^4 f}{dx^4} \cdot \frac{(d-c)^4}{(2l)^4} = \\ &= \frac{-(d-c)^5}{1920} \min_{x \in (c, d)} \frac{d^4 f}{dx^4} \quad (**) \end{aligned}$$

Using (*), we can compute $A_n[f, a, b]$:

$$\begin{aligned} A_n[f, a, b] &= \sum_{i=1}^n A_1[f, x_{i-1}, x_i] = \frac{b-a}{n} \left(f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + \dots + f\left(\frac{x_{n-1}+x_n}{2}\right) \right) + \\ &+ \frac{(b-a)^3}{24n^3} \left(\frac{d^2 f}{dx^2}\left(\frac{x_0+x_1}{2}\right) + \frac{d^2 f}{dx^2}\left(\frac{x_1+x_2}{2}\right) + \dots + \frac{d^2 f}{dx^2}\left(\frac{x_{n-1}+x_n}{2}\right) \right) \end{aligned}$$

$$\begin{aligned} \text{err}(A_1)[f, c, d] &= \frac{d-c}{2l} \text{err}(A_1)\left[x \mapsto f\left(c + \frac{d-c}{2l}x\right), 0, 2l\right] \geq \\ &\geq \left(\frac{d-c}{2l}\right) \left(-\frac{1}{60} l^5 \max_{x \in (0, 2l)} \frac{d^4 f}{dx^4}\left(c + \frac{d-c}{2l}x\right)\right) = \\ &= \frac{d-c}{2l} \cdot \left(-\frac{1}{60} l^5\right) \cdot \frac{(d-c)^4}{16l^4} \cdot \max_{x \in (c, d)} \frac{d^4 f}{dx^4} = \\ &= \frac{-(d-c)^5}{1920} \cdot \max_{x \in (c, d)} \frac{d^4 f}{dx^4} \quad (***) \end{aligned}$$

From $(*)$ and $(**)$ we get that:

$$-\frac{(d-c)^5}{1920} \bar{\Delta}_4 \leq -\frac{(d-c)^5}{1920} \max_{x \in (c,d)} \frac{d^4 f}{dx^4} \leq \text{err}(A_1)[f, c, d] \leq -\frac{(d-c)^5}{1920} \min_{x \in (c,d)} \frac{d^4 f}{dx^4} \leq -\frac{(d-c)^5}{1920} \underline{\Delta}_4$$

$\bar{\Delta}_4 \geq \max_{x \in (c,d)} \frac{d^4 f}{dx^4}$
 $\underline{\Delta}_4 \leq \min_{x \in (c,d)} \frac{d^4 f}{dx^4}$

$$\text{err}(A_n)[f, a, b] = \sum_{i=1}^n \text{err}(M_1)[f, x_{i-1}, x_i]$$

$$-\frac{(b-a)^5}{1920n^5} \bar{\Delta}_4 \leq \text{err}(M_1)[f, x_{i-1}, x_i] \leq -\frac{(b-a)^5}{1920n^5} \underline{\Delta}_4 \quad \Bigg| \quad \sum_{i=1}^n ()$$

$$-\frac{(b-a)^5}{1920n^4} \bar{\Delta}_4 \leq \text{err}(M_n)[f, a, b] \leq -\frac{(b-a)^5}{1920n^4} \underline{\Delta}_4$$

(e) With Simpson's rule we have:

$$S_n[f, a, b] = \frac{b-a}{3n} \left(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots + 4f(x_{n-1}) + f(x_n) \right)$$

$$\frac{(b-a)^5}{180n^4} \underline{\Delta}_4 \leq \text{err}(S_n)[f, a, b] \leq \frac{(b-a)^5}{180n^4} \bar{\Delta}_4$$

Our method:

- $O(n)$ arithmetic operations
- n evaluations of the function f
- n evaluations of the function $\frac{d^2 f}{dx^2}$
- $O(n^{-4})$ error with a factor of $\frac{1}{1920}$

Simpson's rule:

- $O(n)$ arithmetic operations
- $(n+1)$ evaluations of the function
- $O(n^{-4})$ error with a factor of $\frac{1}{180}$

Conclusion:

Considering the fact that our method needs to evaluate the second derivative of f n times, Simpson's rule is definitely faster than our method. In terms of accuracy, because of the factor that is bigger at our method ($1920 > 180$), our method is more accurate than Simpson's rule (slightly, as they have the same complexity $O(n^{-4})$).

$$2.7] \int_0^1 x^2 dx = \left[\frac{x^3}{3} \right]_0^1 = \frac{1}{3}$$

• Estimating it using the Midpoint rule: ($f: [0,1] \rightarrow \mathbb{R}, f(x)=x^2$)

$$M_2[f, 0, 1] = \frac{1}{2} \left(f\left(\frac{0+\frac{1}{2}}{2}\right) + f\left(\frac{\frac{1}{2}+1}{2}\right) \right) = \frac{1}{2} \left(f\left(\frac{1}{4}\right) + f\left(\frac{3}{4}\right) \right) = \frac{1}{2} \left(\frac{1}{16} + \frac{9}{16} \right)$$

$$M_2[f, 0, 1] = \frac{10}{32} = \frac{5}{16}$$

• Estimating it using the Trapezium rule:

$$T_2[f, 0, 1] = \frac{1}{4} \left(f(0) + 2f\left(\frac{1}{2}\right) + f(1) \right) = \frac{1}{4} \left(0 + 2 \cdot \frac{1}{4} + 1 \right) = \frac{1}{4} \cdot \frac{3}{2} = \frac{3}{8}$$

• The error of the Midpoint rule is $\frac{5}{16} - \frac{1}{3} = \frac{15-16}{48} = -\frac{1}{48}$
 • The error of the Trapezium rule is $\frac{3}{8} - \frac{1}{3} = \frac{9-8}{24} = \frac{1}{24}$ } \Rightarrow the Midpoint rule is two times more accurate!

$$\int_0^1 x^4 dx = \left[\frac{x^5}{5} \right]_0^1 = \frac{1}{5}$$

• Estimating it using Simpson's rule: ($g: [0,1] \rightarrow \mathbb{R}, g(x)=x^4$)

$$S_2[g, 0, 1] = \frac{1}{6} \left(g(0) + 4g\left(\frac{1}{2}\right) + g(1) \right) = \frac{1}{6} \left(0 + 4 \cdot \frac{1}{16} + 1 \right) = \frac{1}{6} \cdot \frac{5}{4} = \frac{5}{24}$$

• Estimating it using the method from question 2.6: ($\frac{d^2g}{dx^2} = 12x^2$)

$$A_2[g, 0, 1] = \frac{1}{2} \left(f\left(\frac{1}{4}\right) + f\left(\frac{3}{4}\right) \right) + \frac{1}{192} \left(12 \cdot \frac{1}{16} + 12 \cdot \frac{9}{16} \right)$$

$$A_2[g, 0, 1] = \frac{1}{2} \left(\frac{1}{256} + \frac{81}{256} \right) + \frac{1}{192} \cdot \frac{120}{16} = \frac{1}{2} \cdot \frac{82}{256} + \frac{15}{384} = \frac{41}{256} + \frac{15}{384}$$

$$A_2[g, 0, 1] = \frac{153}{768} = \frac{51}{256}$$

• The error of Simpson's rule is $\frac{5}{24} - \frac{1}{5} = \frac{25-24}{120} = \frac{1}{120}$
 • The error of our method is $\frac{51}{256} - \frac{1}{5} = \frac{255-256}{1280} = -\frac{1}{1280}$ } \Rightarrow Our method is $\frac{32}{3}$ times more accurate!

We have $\frac{d^4g}{dx^4} = 24 \Rightarrow \underline{\Delta_4} = \overline{\Delta_4} = 24$. From the lecture notes, we have

$$24 \cdot \frac{1}{180 \cdot 16} \leq \text{err}(S_2)[g, 0, 1] \leq 24 \cdot \frac{1}{180 \cdot 16} \Rightarrow \text{err}(S_2)[g, 0, 1] = \frac{1}{120}, \text{ as we calculated above.}$$

above.

From question 2.6 we have:

$$-\frac{1}{1920 \cdot 16} \cdot 24 \leq \text{err}(A_2)[g, 0, 1] \leq -\frac{1}{1920 \cdot 16} \cdot 24 \Rightarrow$$

$$\Rightarrow \text{err}(A_2)[g, 0, 1] = -\frac{1}{1280}, \text{ as we calculated above.}$$

2.8. Finally, $\int_0^2 x^{\frac{3}{2}} dx = \left[\frac{2}{5} x^{\frac{5}{2}} \right]_0^2 = \frac{2}{5} \cdot 4\sqrt{2} = \frac{8\sqrt{2}}{5} \approx 2.2627$

Let's also recall Simpson's rule: $(f: [0, 2] \rightarrow \mathbb{R}, f(x) = x^{\frac{3}{2}})$

$$S_n[f, 0, 2] = \frac{2}{3n} (f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots + 4f(x_{n-1}) + f(x_n))$$

Now, the program written in Scala:

object Simpson

```
{
  def Simpson(n: Int): Double = // The function that calculates  $S_n[f, 0, 2]$ 
  {
    var sum = 0.00
    sum = sum + Math.pow(0, 1.5) //  $f(x_0) = f(0)$ 
    for (i <- 1 until n)
    {
      if (i % 2 == 0) sum = sum + 2 * Math.pow(2.0 * i / n, 1.5) //  $4f(1) + 2f(2) + \dots + 4f(n-2) + 2f(n-1)$ 
      else sum = sum + 4 * Math.pow(2.0 * i / n, 1.5)
    }
    sum = sum + Math.pow(2, 1.5) //  $f(x_n) = f(2)$ 
    sum = (2.0 * sum) / (3.0 * n) //  $S_n[f, a, b] = \frac{b-a}{3n} \sum \dots$ 
    sum // We return the result
  }

  def main(args: Array[String]) =
  {
    val trials = scala.io.StdIn.readInt // We try  $2^1, 2^2, \dots, 2^{\text{trials}}$  strips
    var N = 1
    val integral = 2.2627 //  $\int_0^2 x^{\frac{3}{2}} dx$ 
    for (j <- 1 to trials)
    {
      N = N * 2
      val approx = Simpson(N) // the estimate with N strips
      val error = approx - integral
      println("Estimate using " + N + " strips is " + approx + " and the error is " + error)
    }
  }
}
```

We observe that the error converges to a value very close to $4.1699 \cdot 10^{-5}$ even after we use 2^{24} strips. This might be because \overline{D}_n in our case is unbounded (close to 0 it goes to ∞).