Numerical methods in chemistry. Solutions to exercises 4

Problem 1

Applying Laplace transform to both sides of the ODE leads to

$$s^2Y(s) - sy(0) - y'(0) + Y(s) = \frac{6}{s^2+4}.$$

Since $y(0) = 3$ and $y'(0) = 1$ we get

$$(s^2+1)Y(s) = \frac{6}{s^2+4} + 3s + 1,$$

$$Y(s) = \frac{6}{(s^2+4)(s^2+1)} + \frac{3s}{s^2+1} + \frac{1}{s^2+1}.$$

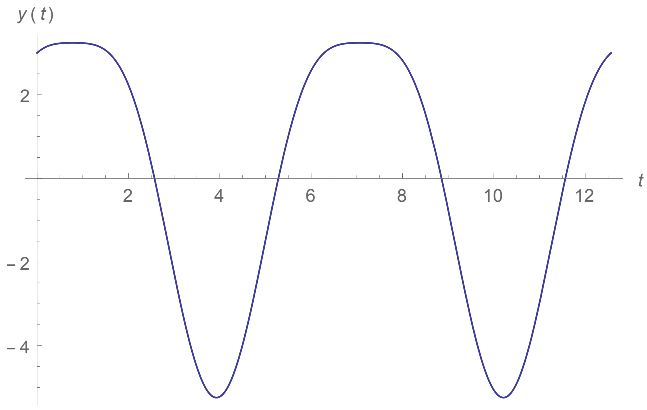
We now use partial fractions on the first summand

$$\frac{6}{(s^2+4)(s^2+1)} = \frac{\alpha}{s^2+4} + \frac{\beta}{s^2+1},$$

$$\begin{cases} \alpha + \beta = 0 \\ \alpha + 4\beta = 6 \end{cases},$$

$$\begin{cases} \alpha = -\beta \\ 3\beta = 6 \end{cases},$$

$$\begin{cases} \alpha = -2 \\ \beta = 2 \end{cases}.$$



Problem 1: Plot of $y(t)$.

We can now write $Y(s)$ as

$$Y(s) = \frac{3}{s^2+1} - \frac{2}{s^2+4} + \frac{3s}{s^2+1}.$$

Applying the inverse Laplace transform leads to

$$y(t) = 3\sin t - \sin 2t + 3\cos t.$$

Problem 2

The transform can be found by straightforward integration

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} h(x)dx = \frac{1}{\pi}\int_0^{\pi} dx = 1,$$

$$a_n \overset{n\neq 0}{=} \frac{1}{\pi}\int_{-\pi}^{\pi} h(x)\cos(nx)dx = \frac{1}{\pi}\int_0^{\pi}\cos(nx)dx = \frac{1}{\pi n}\sin(nx)\Big|_0^{\pi} = 0.$$

(One can see that $a_n = 0$ for $n \neq 0$ also from the fact that $H(x) - 1/2$ is an odd function.) As for the sine coefficients,

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} h(x)\sin(nx)dx = \frac{1}{\pi}\int_0^{\pi}\sin(nx)dx = -\frac{1}{\pi n}\cos(nx)\Big|_0^{\pi} = \frac{1-(-1)^n}{\pi n}.$$

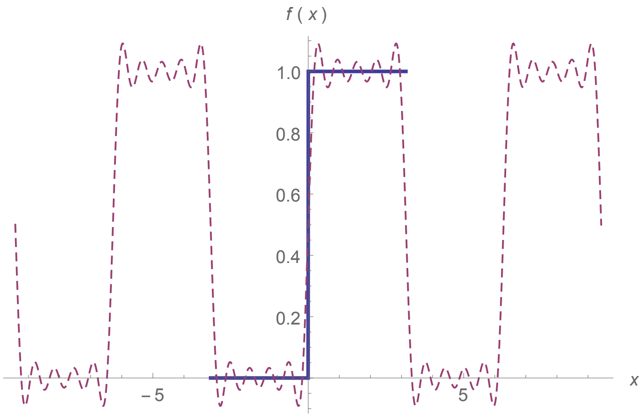
Since $b_n = 0$ for all even n, the resulting Fourier series can be written as

$$h(x) \sim \frac{1}{2} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{\sin[(2n-1)x]}{2n-1}.$$

Since $h(x)$ is continuous at $x = \pi/2$, the Fourier series at $x = \pi/2$ converges to $h(\pi/2)$. Taking $x = \pi/2$ gives

$$\begin{aligned} 1 = h(\pi/2) &= \frac{1}{2} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{\sin\left(\pi n - \frac{\pi}{2}\right)}{2n-1} \\ &= \frac{1}{2} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{2n-1}, \\ \frac{1}{2} &= \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{2n-1}, \quad \text{hence} \\ \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{2n-1} &= \frac{\pi}{4}. \end{aligned}$$

This series is attributed to the Scottish mathematician James Gregory (1638-1675).



Problem 2: Plot of $h(x)$ and its Fourier series truncated at $n = 5$.

Problem 3

The Fourier series can be found using standard integration by parts. Note that since $f(x)$ is an even function, $b_n = 0$ for all $n \in \mathbb{N}$. As for the cosine coefficients a_n, we have

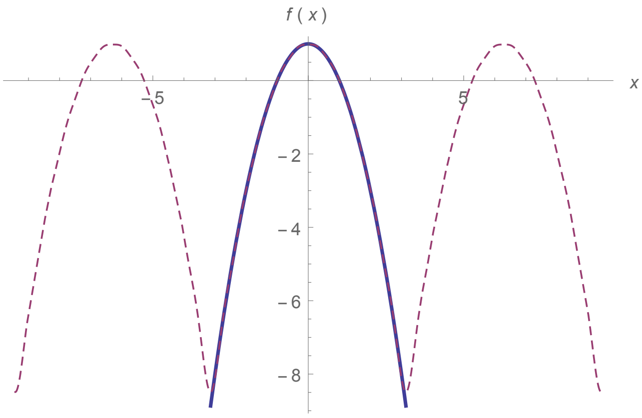
$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi}(1-x^2)dx = \frac{1}{\pi}\left(x|_{-\pi}^{\pi} - \left.\frac{x^3}{3}\right|_{-\pi}^{\pi}\right) = 2\left(1 - \frac{\pi^2}{3}\right).$$

$$\begin{aligned} a_n &\overset{n\neq 0}{=} \frac{1}{\pi}\int_{-\pi}^{\pi}(1-x^2)\cos(nx)dx = \frac{1}{\pi n}\int_{-\pi}^{\pi}(1-x^2)d\sin(nx) = \frac{1}{\pi n}(1-x^2)\sin(nx)\Big|_{-\pi}^{\pi} - \frac{1}{\pi n}\int_{-\pi}^{\pi}\sin(nx)d(1-x^2) \\ &= 0 + \frac{2}{\pi n}\int_{-\pi}^{\pi}x\sin(nx)dx = -\frac{2}{\pi n^2}\int_{-\pi}^{\pi}xd\cos(nx) = -\frac{2}{\pi n^2}x\cos(nx)\Big|_{-\pi}^{\pi} + \frac{2}{\pi n^2}\int_{-\pi}^{\pi}\cos(nx)dx \\ &= -\frac{4(-1)^n}{n^2} + \frac{2}{\pi n^3}\sin(nx)\Big|_{-\pi}^{\pi} = -\frac{4(-1)^n}{n^2}, \end{aligned}$$

The resulting Fourier series is therefore

$$f(x) = 1 - \frac{\pi^2}{3} - 4\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\cos(nx).$$

The equal sign denotes that the Fourier series converges to $f(x)$ for all $x \in \mathbb{R}$ since $f(x)$ is continuous on $\mathbb{R}$.



Problem 3: Plot of $f(x)$ and its Fourier series truncated at $n = 10$.

Problem 4

We find the Fourier series coefficients by straightforward algebra:

$$
\begin{aligned}
a_0 &= \frac{1}{\pi}\int_{-\pi}^{0}\pi^2 dt + \frac{1}{\pi}\int_0^{\pi}(t-\pi)^2 dt = \pi^2 + \frac{(t-\pi)^3}{3\pi}\bigg|_0^{\pi} = \frac{4\pi^2}{3},\\
a_n &\overset{n\neq 0}{=} \frac{1}{\pi}\int_{-\pi}^{0}\pi^2\cos(nt)dt + \frac{1}{\pi}\int_0^{\pi}(t-\pi)^2\cos(nt)dt = \frac{\pi}{n}\sin(nt)\bigg|_{-\pi}^{0} + \frac{1}{\pi n}\int_0^{\pi}(t-\pi)^2 d\sin(nt)\\
&= \frac{1}{\pi n}(t-\pi)^2\sin(nt)\bigg|_0^{\pi} - \frac{1}{\pi n}\int_0^{\pi}\sin(nt)d(t-\pi)^2 = -\frac{2}{\pi n}\int_0^{\pi}(t-\pi)\sin(nt)dt = \frac{2}{\pi n^2}\int_0^{\pi}(t-\pi)d\cos(nt)\\
&= \frac{2}{\pi n^2}(t-\pi)\cos(nt)\bigg|_0^{\pi} - \frac{2}{\pi n^2}\int_0^{\pi}\cos(nt)d(t-\pi) = \frac{2}{n^2} - \frac{2}{\pi n^3}\sin(nt)\bigg|_0^{\pi} = \frac{2}{n^2},\\
b_n &= \frac{1}{\pi}\int_{-\pi}^{0}\pi^2\sin(nt)dt + \frac{1}{\pi}\int_0^{\pi}(t-\pi)^2\sin(nt)dt = -\frac{\pi}{n}\cos(nt)\bigg|_{-\pi}^{0} - \frac{1}{\pi n}\int_0^{\pi}(t-\pi)^2 d\cos(nt)\\
&= -\frac{\pi(1-(-1)^n)}{n} - \frac{1}{\pi n}(t-\pi)^2\cos(nt)\bigg|_0^{\pi} + \frac{1}{\pi n}\int_0^{\pi}\cos(nt)d(t-\pi)^2\\
&= -\frac{(1-(-1)^n)\pi}{n} + \frac{\pi}{n} + \frac{2}{\pi n}\int_0^{\pi}(t-\pi)\cos(nt)dt = \frac{(-1)^n\pi}{n} + \frac{2}{\pi n^2}\int_0^{\pi}(t-\pi)d\sin(nt)\\
&= \frac{(-1)^n\pi}{n} + \frac{2}{\pi n^2}(t-\pi)\sin(nt)\bigg|_0^{\pi} - \frac{2}{\pi n^2}\int_0^{\pi}\sin(nt)d(t-\pi)\\
&= \frac{(-1)^n\pi}{n} + \frac{2}{\pi n^3}\cos(nt)\bigg|_0^{\pi} = \frac{(-1)^n\pi}{n} + \frac{2[(-1)^n-1]}{\pi n^3}.
\end{aligned}
$$

We can now write the Fourier series as

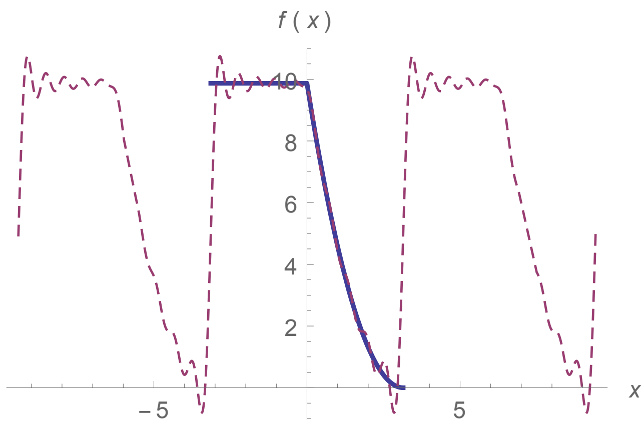
$$
\frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\left[\frac{2}{n^2}\cos(nt) + \frac{(-1)^n\pi}{n}\sin(nt)\right] - \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{\sin[(2n-1)t]}{(2n-1)^3}.
$$

Since $f(t)$ is continuous at $t=0$, the Fourier series at $t=0$ converges to $f(0)$. Therefore, to find the first series we simply take $t=0$ and obtain

$$
\begin{aligned}
\pi^2 = f(0) &= \frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\frac{2}{n^2}, \text{ hence}\\
\sum_{n=1}^{\infty}\frac{1}{n^2} &= \frac{\pi^2}{6}.
\end{aligned}
$$

The value of the second series can be obtained by taking $t=\pi$. However, since the function $f(t)$ is not continuous at $t=\pi$ [the the limit from the left $(t\to\pi_+)$ being π^2 and the limit from the right $(t\to\pi_-)$ being 0], we need to use Dirichlet's theorem to find the sum of the Fourier series. The result is

$$
\begin{aligned}
\frac{1}{2}\left[f(\pi_+)+f(\pi_-)\right] &= \frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\frac{2}{n^2}(-1)^n,\\
\frac{\pi^2}{2} &= \frac{2\pi^2}{3} + \sum_{n=1}^{\infty}\frac{2}{n^2}(-1)^n, \text{ hence}\\
\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2} &= \frac{\pi^2}{12}.
\end{aligned}
$$



Problem 4: Plot of $f(x)$ and its Fourier series truncated at $n=10$.