Assignment 10AB

In this problem we consider a 1D metal rod of length L, where the temperature distribution $T(t,x)$ at $t=0$ is given by a finite sum of sine modes:

$$T(0,x) = \sum_{n=1}^{N} c_n \sin\left(\frac{n\pi x}{L}\right) . \tag{1}$$

The temperature profile evolves according to the heat equation:

$$\frac{\partial T(t,x)}{\partial t} = \alpha \frac{\partial^2 T(t,x)}{\partial x^2} , \tag{2}$$

where α is the thermal diffusivity. The boundary conditions are assumed to be the following:

$$T(t,0) = 0, \quad T(t,L) = 0 . \tag{3}$$

The corresponding exact solution for the temperature at any time t is given by:

$$T(t,x) = \sum_{n=1}^{N} c_n e^{-\alpha\left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi x}{L}\right) . \tag{4}$$

Since the Fourier modes with higher n are suppressed exponentially, we expect that the temperature profile is dominated by only a few Fourier components after enough time (regardless of the temperature profile of the rod at $t = 0$). **In this assignment, you will analyze the time evolution of the system and apply Gaussian Process Regression (GPR) to reconstruct the temperature profile at different times, leveraging this general feature of the heat equation.**

Hint: Computing the inverse of a matrix is a key step in this assignment. To invert matrices you may use the numerical linear algebra Python library `numpy.linalg.inv`. For example, given a matrix M, its inverse can be computed efficiently using:

```
import numpy as np

M = np.array([[4, 7], [2, 6]])  # Example matrix
M_inv = np.linalg.inv(M)        # Compute the inverse

print(M_inv)
```

- **Problem 1 (200 points):** Gaussian Process Regression with Physics-Informed Prior

  To proceed, you may adopt the following parameter choices and initial condition generator:

```
# Parameters
L = 1.0          # Length of the rod
alpha = 0.01     # Thermal diffusivity
N_modes = 10     # Number of sine modes in the expansion

# Use the specified random generator
rng = np.random.default_rng(42)  # PCG64-based generator with fixed seed

# Generate random Fourier coefficients
c_n = rng.uniform(-1, 1, N_modes)

# Function to compute the initial temperature profile
def initial_temperature(x, L, c_n):
    return sum(c_n[n] * np.sin((n+1) * np.pi * x / L) for n in range(len(c_n)))
```

  (a) Compute the prior covariance matrix $A_{ss'}$, using the physics-informed choice:

$$A_{ss'} = e^{\alpha\left(\frac{s\pi}{L}\right)^2 t}\delta_{ss'}\,. \tag{5}$$

  Compute $A_{ss'}^{-1}$ and use it to construct the kernel function:

$$K(x,x') = \sum_{s=1}^{N} A_{ss}^{-1}\sin\left(\frac{s\pi x}{L}\right)\sin\left(\frac{s\pi x'}{L}\right)\,. \tag{6}$$

  Compute and plot $K(x,x')$ for times $t = 0, 0.25, 0.5, 0.75, 1, 2$.

  Note: You will be asked to physically motivate this choice of $A_{ss'}$ in Question (d).

  (b) Compute the covariance matrix $\bar{K}_{\alpha\beta}$ for the training data, incorporating the measurement uncertainty σ:

$$\bar{K}_{\alpha\beta} = K(x_\alpha, x_\beta) + \sigma^2\delta_{\alpha\beta}\,. \tag{7}$$

  The measurements correspond to temperature values extracted from the provided function at:

$$x_\alpha = L/6, L/3, L/2, 2L/3, 5L/6\,. \tag{8}$$

  Denoting these measurements as $T_\alpha \equiv T(t, x_\alpha)$, with measurement uncertainty $\sigma = 0.01$, compute the mean prediction:

$$\langle T(x)\rangle = \sum_{\alpha,\beta} K(x, x_\alpha)\bar{K}_{\alpha\beta}^{-1}T_\beta\,, \tag{9}$$

  and the standard deviation:

$$\sigma_{\text{post}}^2(x) = K(x,x) - \sum_{\alpha,\beta} K(x, x_\alpha)\bar{K}_{\alpha\beta}^{-1}K(x_\beta, x)\,. \tag{10}$$

  (c) Perform the GPR reconstruction for the same times as the kernel calculations: $t = 0$, 0.25, 0.5, 0.75, 1, 2. Plot the predicted mean temperature profile $\langle T(x)\rangle$ for each case along with the standard deviation confidence interval (error bars). Compare the reconstructed function to the true solution of the heat equation at the corresponding time.

  Note: You are allowed to use any language model of choice (Chat-GPT, Claude, DeepSeek, etc...) to display the standard deviation as a shaded area around the GPR prediction, in a similar fashion as in the plots of the lecture notes. ***Note that the use of language models is permitted exclusively for learning how to edit the plot nicely, but not for solving the problem.***

(d) In the Jupyter Notebook, provide a brief explanation in markdown discussing the role of the prior covariance matrix $A_{ss'}$ in the Gaussian Process Regression model. Explain how the structure of $A_{ss'}$ encodes the expected physical behavior of the system and why this choice is justified based on the heat equation. Additionally, comment on the agreement between the reconstructed function and the actual temperature profile as a function of time.

Note: The kernel function and related quantities depend on the time parameter t, but for simplicity, this dependence is omitted in the notation.