Math 304, Spring 2020 - Homework 1

February 18, 2020

Due on March 4th 2020, Wednesday by 17:30

The specific heat capacity of a substance corresponds to the amount of heat needed per unit mass to increase its temperature by one unit. This homework asks you to estimate the the specific heat capacity $C(T)$ (in Joule / (Kelvin·Mole)) of graphite, a crystalline form of the atom carbon, as a function of temperature T (in Kelvin) by employing polynomial interpolation.

A chemist measures (in the units specified in the previous paragraph) the specific heat capacity, as well as the rate-of-change in the specific heat capacity (i.e., the derivative of the specific heat capacity), of graphite at various temperatures in the interval $[300, 600]$. The data is provided together with this homework; see `specheat_data.mat`. This data consists of 25 triplets of the form (T_j, C_j, D_j) for $j = 1, \ldots, 25$, where T_j represents the temperature, C_j is the measured specific heat capacity, D_j is the measured derivative of the specific heat capacity at temperature T_j. A plot of the data is given in Figure 1 below.

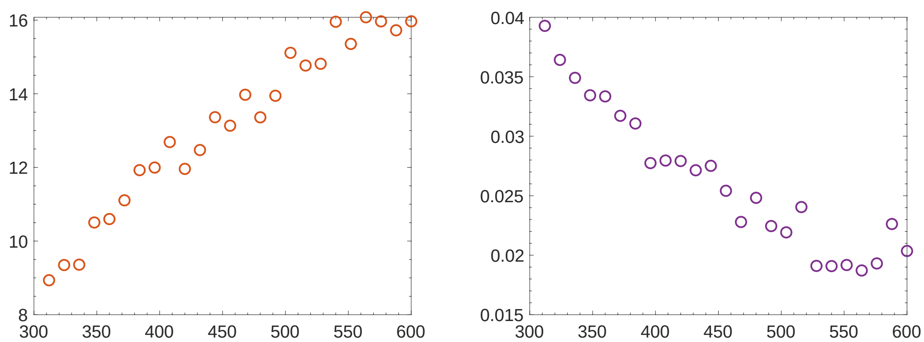

Figure 1: The plot of the data (T_j, C_j, D_j) for $j = 1, \ldots, 25$, where the horizontal axis is the temperature, whereas the vertical axis corresponds to the specific heat capacity on the left, and its derivative on the right. **(Left)** (T_j, C_j) for $j = 1, \ldots, 25$. **(Right)** (T_j, D_j) for $j = 1, \ldots, 25$.

As discussed in class there exists a unique polynomial $C(T)$ of degree $n-1$ such that

$$C(T_{k_j}) = C_{k_j} \quad \text{for } j = 1, \dots, n,$$

where $k_1, \dots, k_n \in \{1, \dots, 25\}$ are distinct integers. For instance, the unique polynomial $C(T)$ of degree 5 such that $C(T_{4j}) = C_{4j}$ for $j = 1, \dots, 6$ is plotted below, where the interpolation points are marked with black crosses.

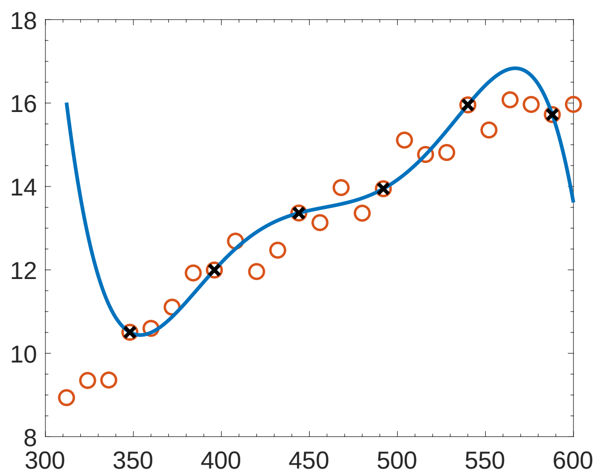

Figure 2: The blue curve is the graph of the unique polynomial $C(T)$ of degree 5 such that $C(T_{4j}) = C_{4j}$ for $j = 1, \dots, 6$.

In all parts below, you can use the Matlab routines discussed in class and made available on the course webpage. In each part, you must include the print-outs of the Matlab commands you used, and/or the Matlab routines you implemented, in addition to what is asked in the question.

1. Find the cubic polynomial through the points

$$(T_6, C_6), (T_{12}, C_{12}), (T_{18}, C_{18}), (T_{24}, C_{24})$$

using the Vandermonde matrix based approach, in particular by solving a linear system whose coefficient matrix is a Vandermonde matrix.

Provide a plot of the cubic polynomial that you computed, similar to the plot in Figure 2. Provide also precisely the coefficients of the polynomial you computed.

2. Find the polynomial of degree 7 through the points

$$(T_{3j}, C_{3j}) \qquad j = 1, \dots, 8$$

using the Lagrange interpolation. Again provide a plot of the computed polynomial (similar to Figure 2), as well as the coefficients of the polynomial.

3. Hermite interpolation involves not only the interpolation of the function values, but also the interpolation of the derivatives. For instance, there exists a unique polynomial $C(T)$ of degree $2n-1$ such that

$$C(T_{k_j}) = C_{k_j} \quad \text{and} \quad C'(T_{k_j}) = D_{k_j} \quad \text{for } j = 1, \dots, n, \tag{0.1}$$

where again $k_1, \dots, k_n \in \{1, \dots, 25\}$ are distinct integers.

Devise a generalization of the Vandermonde matrix based approach discussed in the class for Hermite interpolation so that the polynomial $C(T)$ satisfies (0.1) for a specified integer n and specified $k_1, \dots, k_n \in \{1, \dots, 25\}$. In particular, you must set up a linear system

$$Ax \;=\; b$$

where A is a $2n \times 2n$ Vandermonde-like matrix, then solve the linear system using the command `x = A\b` in Matlab.

Implement your method in Matlab. Then use it to find the unique polynomial $C(T)$ of degree 5 such that

$$C(T_{8j}) = C_{8j} \quad \text{and} \quad C'(T_{8j}) = D_{8j}$$

for $j = 1, 2, 3$. Provide the plot of the computed $C(T)$ following the practice in Figure 2. Additionally, provide the plot of $C'(T)$ again following the practice in Figure 2, but by employing the data points for the derivatives, i.e., by employing the points on the right-hand side of Figure 1 rather than the left-hand side. Also include the coefficients of the computed polynomial.

4. It is also possible to perform Hermite interpolation using the Newton form. Defining $x_1, \dots, x_{2n}$ by $x_{2j-1} = x_{2j} = T_{k_j}$, it can be shown that the polynomial of degree $2n-1$ satisfying (0.1) can be expressed as

$$C(T) = c_1 + c_2\phi_2(T) + c_3\phi_3(T) + \cdots + c_n\phi_n(T)$$

where $c_1 = f(x_1)$ and

$$\phi_j(T) = (T - x_1)(T - x_2)\dots(T - x_{j-1}), \quad c_j = f[x_1, x_2, \dots, x_j]$$

for $j = 2, 3, \dots, n$.

The divided differences are still defined nearly as discussed in the class, that is, for $j > i$, we have

$$f[x_i, \dots, x_j] \;:=\; \frac{f[x_{i+1}, \dots, x_j] - f[x_i, \dots, x_{j-1}]}{x_j - x_i} \quad \text{and} \quad f[x_i] := f(x_i)$$

with the only exception

$$f[x_i, x_{i+1}] := \begin{cases} f'(x_i) & \text{if } x_i = x_{i+1}, \\ \dfrac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} & \text{if } x_i \neq x_{i+1}. \end{cases}$$

Implement the Newton form in Matlab. Use it to find the unique polynomial $C(T)$ of degree 9 such that

$$C(T_{5j}) = C_{5j} \quad \text{and} \quad C'(T_{5j}) = D_{5j}$$

for $j = 1, 2, 3, 4, 5$. Once again provide the plots of the computed $C(T)$ and $C'(T)$, as well as the coefficients of $C(T)$.