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Numerical Methods - pset 4

1 Problem 1

1.1 Part A

`Part A` of `problem 1` requires the calculation of the Pade approximations $P[3,4]$ and $P[2,5]$ for the function $f(x) = e^x$. To aid these calculations, Mathematica was used in calculating the Taylor expansion and derivatives.

A Pade expansion $R_N(x)$ takes the following form:

$$f(x) = R_N(x) \equiv \frac{P_n(x)}{Q_m(x)} = \frac{a_0 + a_1 x + a_2 x^2 + ... + a_n x^n}{1 + b_1 x + b_2 x^2 + ... + b_m x^m}$$

with $N = n + m$.

Calculating a Pade approximation $R_{3,4}(x)$ of $f(x)$ requires first calculating the Maclaurin series of degree $N = 3 + 4 = 2 + 5 = 7$ for $f(x)$ (Taylor series about $x = 0$).

$$\begin{aligned} f(x) &= e^x \\ T_7(f(x)) &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120} + \frac{x^6}{720} + \frac{x^7}{5040} \end{aligned}$$

We then create the difference

$$\begin{aligned} T_7(x) - R_{3,m}(x) &= 0 \\ \Rightarrow (T_7(x)) - \frac{a_0 + a_1 x + a_2 x^2 + a_3 x^3}{1 + b_1 x + b_2 x^2 + ... + b_m x^m} &= 0 \end{aligned}$$

Multipying out the denominator thus leads to

$$\frac{1}{1 + ... + b_m x^m}\left[T_7(x)(1 + b_1 x + .. + b_m x^m) - \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)\right] = 0.$$

from which it follows

$$T_7(x)(1 + b_1 x + .. + b_m x^m) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

Setting $m = 4$ for the Pade approximation $P[3,4]$ results in

$$T_7(x)\left(1 + b_1 x + b_2 x^2 + b_3 x^3 + b_4 x^4\right) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

Multiplying out these polynomials and combining like terms leads the following system of eight equations:

$$\begin{aligned}
0 &= 1 - a_0 \\
0 &= 1 + b_1 - a_1 \\
0 &= \frac{1}{2} + b_1 + b_2 - a_2 \\
0 &= \frac{1}{6} + \frac{b_1}{2} + b_2 + b_3 - a_3 \\
0 &= \frac{1}{24} + \frac{b_1}{6} + \frac{b_2}{2} + b_3 + b_4 \\
0 &= \frac{1}{120} + \frac{b_1}{4} + \frac{b_2}{6} + \frac{b_3}{2} + b_4 \\
0 &= \frac{1}{720} + \frac{b_1}{120} + \frac{b_2}{24} + \frac{b_3}{6} + \frac{b_4}{2} \\
0 &= \frac{1}{5040} + \frac{b_1}{720} + \frac{b_2}{120} + \frac{b_3}{24} + \frac{b_4}{6}
\end{aligned}$$

Solving this system of equations using Mathematica yields the expected values for a and b:

$$\begin{aligned}
a_0 &= 1 \\
a_1 &= \frac{3}{7} \\
a_2 &= \frac{1}{14} \\
a_3 &= \frac{1}{210} \\
b_1 &= -\frac{4}{7} \\
b_2 &= \frac{1}{7} \\
b_3 &= -\frac{2}{105} \\
b_4 &= \frac{1}{840}
\end{aligned}$$

These values match the given Pade approximation, proving the relation as desired.
The process for calculating $P[2,5]$ is analogous:

$$\begin{aligned}
T_7(x)(1 + b_1x + .. + b_mx^m) &= a_0 + a_1x + a_2x^2. \\
\Rightarrow T_7(x)\big(1 + b_1x + b_2x^2 + b_3x^3 + b_4x^4 + b_5x^5\big) &= a_0 + a_1x + a_2x^2.
\end{aligned}$$

The resulting system of equations is:

$$
\begin{aligned}
0 &= 1 - a_0 \\
0 &= 1 + b_1 - a_1 \\
0 &= \frac{1}{2} + b_1 + b_2 - a_2 \\
0 &= \frac{1}{6} + \frac{b_1}{2} + b_2 + b_3 \\
0 &= \frac{1}{24} + \frac{b_1}{6} + \frac{b_2}{2} + b_3 + b_4 \\
0 &= \frac{1}{120} + \frac{b_1}{24} + \frac{b_2}{6} + \frac{b_3}{2} + b_4 + b_5 \\
0 &= \frac{1}{720} + \frac{b_1}{120} + \frac{b_2}{24} + \frac{b_3}{6} + \frac{b_4}{2} + b_5 \\
0 &= \frac{1}{5040} + \frac{b_1}{720} + \frac{b_2}{120} + \frac{b_3}{24} + \frac{b_4}{6} + \frac{b_5}{2}
\end{aligned}
$$

Solving this system of equations using Mathematica once again yields the desired values for a and b:

$$
\begin{aligned}
a_0 &= 1 \\
a_1 &= \frac{2}{7} \\
a_2 &= \frac{1}{42} \\
b_1 &= -\frac{5}{7} \\
b_2 &= \frac{5}{21} \\
b_3 &= -\frac{1}{21} \\
b_4 &= \frac{1}{168} \\
b_5 &= -\frac{1}{2520}
\end{aligned}
$$

All three methods yield at least six decimal places of accuracy at $x = 0.5$. This changes quickly after about $x = 3.5$ at which point the functions take on very different values.

At $x = 2$ all three functions agree to at least 2 decimal places. At $x = 5$, only the taylor approximation has the correct order of magnitude compared to the true value of the function and $P[2, 5]$ is even negative.

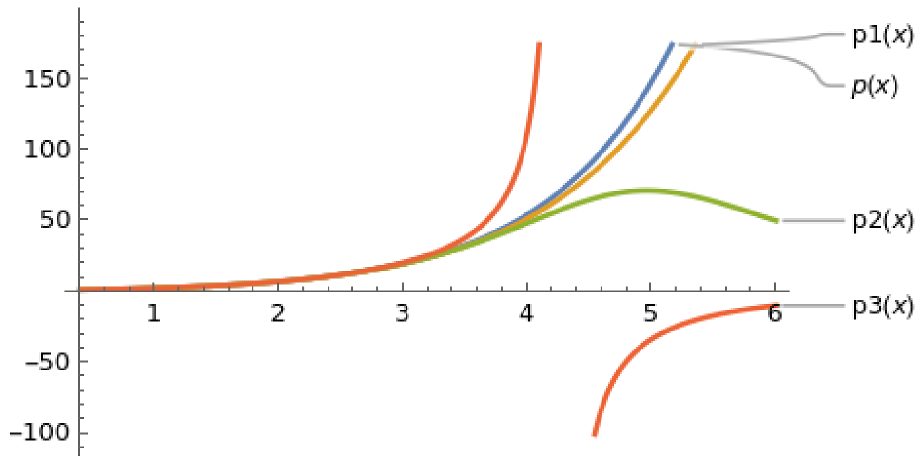

Figure 1: Graph of the original exponential function and the three different approximations

2 Problem 2

For `problem 2` we are given four data points (x, y) and asked to find a third degree polynomial connecting these points.

The provided table (seen below) also contains the calculated forward differences for the values.

k	x_k	$f(x_k)$	$\Delta f(x_k)$	$\Delta^2 f(x_k)$	$\Delta^3 f(x_k)$
0	4	1			
			2		
1	6	3		3	
			5		4
2	8	8		7	
			12		
3	10	20			

Given that these values are in order and equally spaced, we can use the following simplified formula to calcuate the Newton forward differences polynomial from the given values:

$$P(x) = \sum_{i=0}^{n} \binom{s}{i} \Delta^i f_0,$$

with h being the spacing between the x-values and $s = \frac{x - x_0}{h}$.

We can thus use the following expression to obtain the desired polynomial of degree three:

$$P_3(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_0$$

We insert $h = 2$ and the above expression for s, as well as the forward finite differences to obtain the following (calculations done using Mathematica):

$$P_3(x) = \frac{x^3}{12} - \frac{9x^2}{8} + \frac{71x}{12} - 10,$$

which matches the given expression.