AMT Homework 6 Supplement

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The purpose of this supplement is to illustrate some of the techniques used to fit data to a functional equation and approximate the behavior of oscillatory systems, either using the second integral or by making an analogy with simple harmonic motion.

1. Physical arguments give you reason to believe that the data you obtain from an experiment follow a cubic polynomial. The experiment gives data shown in the table:

x	0.3	0.7	1.4	2.3	2.8	3.4	3.8
y	4.5	5.9	3.5	2.9	0.9	1.6	4.1
σ_y	0.1	0.4	1.5	1.6	0.1	0.7	1.1

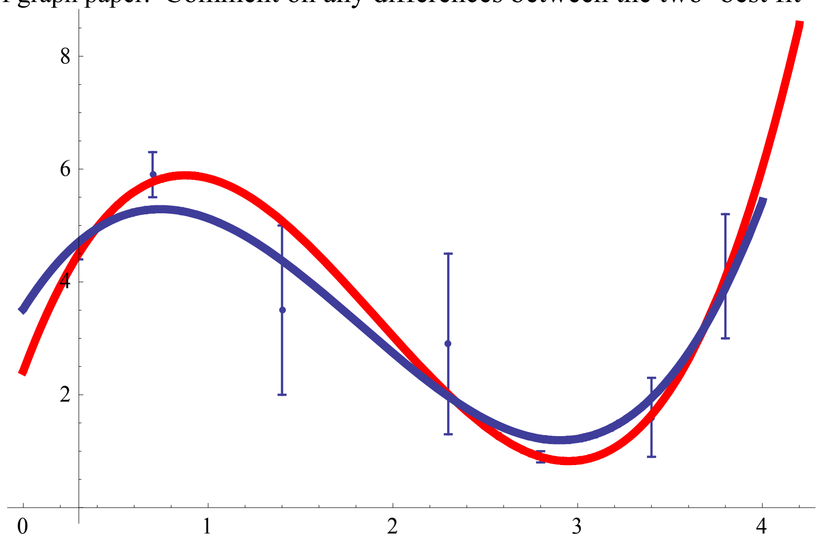
(a) Write an expression for χ^2, assuming a general cubic form for y.

(b) Determine the equations satisfied by the cubic polynomial coefficients that yield an extremal value of χ^2.

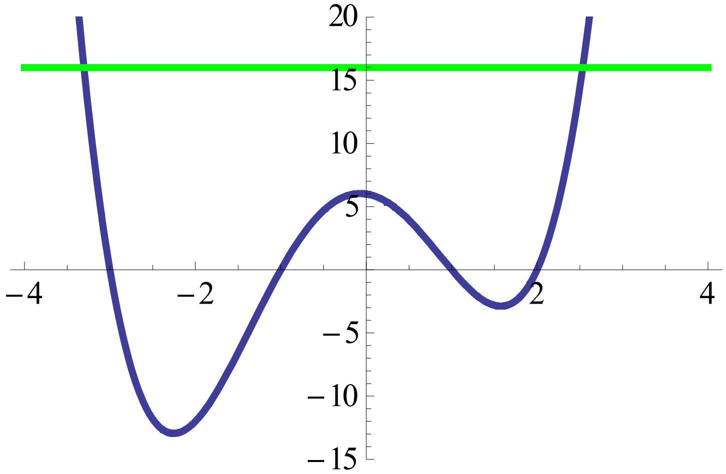
(c) Solve the equations you obtained in part (b) for the coefficients of the polynomial that minimizes χ^2. Compare the resulting polynomial with the one obtained directly from the cubic fitting function on your calculator.
The fit gives $y = 0.81x^3 - 4.43x^2 + 5.23x + 3.517$.

(d) The values of y determined from experiment are not exact; there are errors associated with each of them that are given in the table in the row labeled σ_y. You intend to re-compute the coefficients of your cubic, this time associating a stronger weight to the values with smaller errors. In this vein, you define a modified $\tilde{\chi}^2$ by weighting with the inverse of the square of the error. Write down an expression for $\tilde{\chi}^2$ and obtain the coefficients of the cubic polynomial that minimizes it. Hint: Use a spreadsheet to obtain your coefficient sums… there are 11 of them!
The modified fit gives $y = 1.13x^3 - 6.51x^2 + 8.79x + 2.42$.

(e) Graph both of your best fit polynomials along with the data (include error bars!) on a piece of graph paper. Comment on any differences between the two 'best fit' cubics.



2. A particle with a mass of 2 kg moves in one dimension under the influence of a potential given by $U(x) = x^4 + x^3 - 7x^2 - x + 6$, where U is in joules when x is given in meters. In the following, all values are given in SI units. Give answers correct to three decimal places.
Ok. For this problem, the VERY FIRST thing you need to do is produce a graph:



Now that that's out of the way, we can understand what the questions mean…

(a) The particle is found at $x = 1.5$ at some time with a total energy of 0. How fast is it moving? What is the maximum distance it can go to the left? To the right?

Total energy is zero, so this is represented by the x-axis. The object will move back and forth between $x = 1$ and 2. Its current speed is given by conservation of energy, $E = 0 = \frac{1}{2}mv^2 + U(x) \quad \Rightarrow \quad v = \sqrt{-2U/m}$. At $x = 1.5$, its speed is 1.677 meters per second. It can go a maximum of 0.5 meters to the left or right of its initial location.

(b) Write an integral expression for the period of the particle's motion under the assumptions of part (a). Determine an approximate value of this period using the method shown in class.

$$T = \sqrt{2m}\int_{x_{\min}}^{x_{\max}} \frac{dx}{\sqrt{E - U(x)}} = 2\int_1^2 \frac{dx}{\sqrt{-U(x)}}$$
$$\approx 2\left[\int_{1.01}^{1.99} \frac{dx}{\sqrt{-U(x)}} + 2\sqrt{\frac{0.01}{-U'(1)}} + 2\sqrt{\frac{0.01}{U'(2)}}\right].$$

The value of this approximation is 1.89708, while the exact value is 1.8974006… .

(c) The particle is found at x = -3 moving at 4 meters per second at some time. What is its total energy? How far to the right can it go? To the left? At what value of x will it be moving the fastest?

The total energy is clearly $\frac{1}{2}mv^2 + U(x) = 4^2 + U(-3) = 16$, indicated by the green line in the diagram above, so the turning points are the roots of the equation $U(x) = 16$, $x = -3.30416$ and 2.53357. There are clearly only two roots, as is obvious from the diagram, so the object will move back and forth between them. It can go 0.30416 meters to the left and 5.53357 meters to the right. It will be moving the fastest at the deepest minimum, $x = -2.25375$. Its speed there is 5.38047 meters per second.

(d) Write an integral expression for the period of motion of the object under the assumptions given in part (c), and determine its value using the method shown in class.

$$T = \sqrt{2m}\int_{x_{\min}}^{x_{\max}} \frac{dx}{\sqrt{E-U(x)}} = 2\int_{-3.30416}^{2.53357} \frac{dx}{\sqrt{16-U(x)}}$$
$$\approx 2\left[\int_{-3.29416}^{2.52357} \frac{dx}{\sqrt{16-U(x)}} + 2\sqrt{\frac{0.01}{-U'(-3.30416)}} + 2\sqrt{\frac{0.01}{U'(2.53357)}}\right].$$

The value is 3.19334 seconds, while exact is 3.19209.

3. The Lennard-Jones, or 6-12, potential is used extensively to model the vibrations of correlated pairs of molecules. It is empirically based on the fact that the potential experienced by these molecules generates a repulsive force when the molecules get too close because of the mutual repulsion of the electron clouds and generates an attractive force when the molecules are far apart because of small molecular dipole effects and London forces (quantum dipole effects). The form of the potential is

$$U(r) = \frac{A}{r^{12}} - \frac{B}{r^6},$$

where r is the molecular separation and A and B are empirically determined constants.

(a) Determine the equilibrium value r_0 of r for this system and show that the potential can be written in dimensionless form as

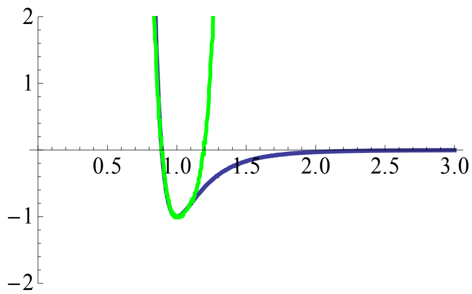
$$U(\xi r_0) = U_0\left(\xi^{-12} - 2\xi^{-6}\right),$$

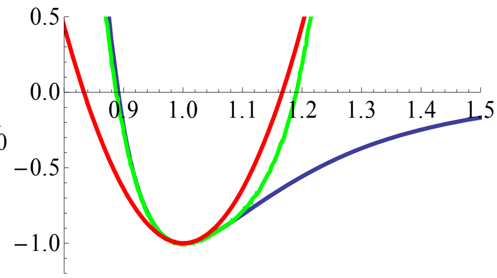
where $\xi = r/r_0$ and U_0 is some combination of A, B, and r_0. Determine U_0 in terms of these constants.

$U'(r_0) = 0 \Rightarrow$ equilibrium is at $r_0 = \sqrt[6]{2A/B}$. Plugging in gives $U_0 = B^2/4A$.

(b) Expand $U(\xi r_0)$ in a Taylor series about $\xi = 1$, keeping terms up to $O\left[(\xi-1)^4\right]$. Graph the potential and your polynomial approximation to show that your approximation follows the curve in the appropriate manner (you may take $U_0 = 1$ in your graph).

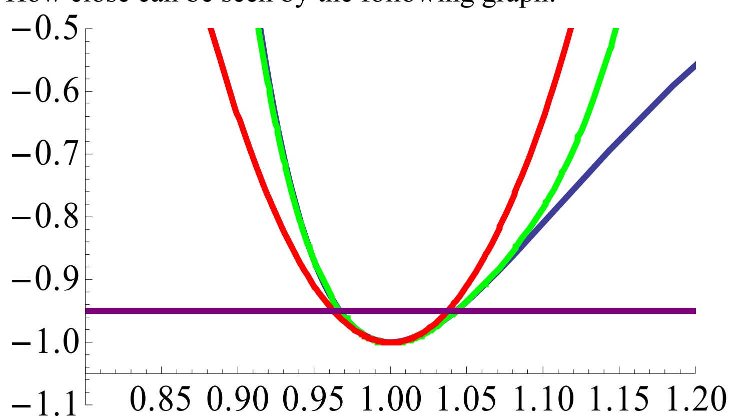
$U(\xi r_0) = U_0\left[-1 + 36(\xi-1)^2 - 252(\xi-1)^3 + 1113(\xi-1)^4 + \cdots\right]$. In the graph, the green curve is the approximation and the blue curve is the exact.





(c) If the total energy of the molecular system is only slightly greater than $-U_0$, argue that only the leading two nonzero terms of your expansion in (b) are important. Obtain the period of small oscillations about the equilibrium $\xi = 1$ in this case by analogy to another important physical system we have studied. Take the relevant mass (called the *reduced mass* of the system) as m. Argue that these *small amplitude* oscillations have a period that is independent of the total energy E.

If we are *very* close to the minimum, the red curve, containing only the constant and the quadratic terms of our polynomial expansion, lies fairly close to the blue curve. It is NOT a very good approximation, as evidenced by the above graph, but it works when we are very close to the minimum. How close can be seen by the following graph:



Thus, we expect the quadratic approximation to be ‘ok’ when the total energy is smaller than about $-0.95\,U_0$, marked with the horizontal purple line. Happily, the quadratic approximation is simply simple harmonic motion (this is *always* the case with a quadratic approximation). The period is therefore expected to be independent of the amplitude and have the value $T_{SHM}=2\pi\sqrt{m/k}$, where k is the 'spring constant'. Our quadratic term is $36\,U_0(\xi-1)^2=36\,U_0\left(\frac{r-r_0}{r_0}\right)^2$, to be compared with $\frac{1}{2}k(x-x_0)^2$. Our spring constant is therefore $72U_0/r_0^2$ and the period is $2\pi\sqrt{mr_0^2/72U_0}$.

(d) Write down an expression for the period of oscillation associated with a system with total energy $E=-U_0+\varepsilon U_0$ and make a table comparing the period you obtained in (c) with the exact period (obtained by numerical integration of your expression) for values of $\varepsilon = 0.01,\ 0.1,$ and 0.5. Your expressions for the period should contain the constants $U_0, r_0,$ and m, along with a numerical value from the integration. Note that each of these integrals is improper because of a vertical asymptote in the integrand at each endpoint. For this reason, you should regularize the integrals in the manner shown in class. Cut off the integration 0.01 units away from each endpoint, and include your corrections.

$$T=\sqrt{2m}\int_{\xi_{\min}}^{\xi_{\max}}\frac{r_0\,d\xi}{\sqrt{U_0\left(-1+\varepsilon-\xi^{-12}+2\xi^{-6}\right)}}=\sqrt{\frac{2mr_0^2}{U_0}}\int_{\xi_{\min}}^{\xi_{\max}}\frac{d\xi}{\sqrt{\varepsilon-\left(1-\xi^{-6}\right)^2}}$$

$$\approx\sqrt{\frac{2mr_0^2}{U_0}}\left[\int_{\xi_{\min}+\delta}^{\xi_{\max}-\delta}\frac{d\xi}{\sqrt{\varepsilon-\left(1-\xi^{-6}\right)^2}}+2\sqrt{\frac{\delta}{-f'(\xi_{\min})}}+2\sqrt{\frac{\delta}{f'(\xi_{\max})}}\right],$$

where I have defined $f(\xi)=\left(1-\xi^{-6}\right)^2$. We can, amazingly, solve exactly for the maximum and minimum values of ξ: $\xi_{\min}=\left(1+\sqrt{\varepsilon}\right)^{-1/6}$ and $\xi_{\max}=\left(1-\sqrt{\varepsilon}\right)^{-1/6}$. This doesn't make the derivatives 'beautiful', though, so we'll resort to numerics (we'll have to do this anyway for the integral…). The table is below.

ε	$T_{exact}/\sqrt{2mr_0^2/U_0}$	$T_{approx}/\sqrt{2mr_0^2/U_0}$	$T_{SHM}/\sqrt{2mr_0^2/U_0}$
0.01	0.526935	0.505772	0.5236
0.1	0.55968	0.5565	0.5236
0.5	0.8135	0.8129	0.5236

The simple harmonic approximation is clearly quite good when the object is very close to its equilibrium, but horribly inaccurate when the object is allowed to stray farther from the minimum. Note that the anomalously poor value given by our approximation when $\varepsilon=0.01$ is due to our choice of cut off as 0.01. The minimum and maximum values of ξ in this case are 0.98424 and 1.01772, so we are cutting off more than half the integral! Cutting off at 0.001 instead gives the much more respectable value 0.526353.