HW #5 (Feb.23, 2016): Computational Physics

Deadline: Mar.1, 2016 5pm EST

1. Write a program for fitting hypothetical Millikan's oil-drop experimental data shown in Table 1 and Fig.1 to a linear function, $e_n = ne_0 + \Delta e$, by using the least-squares fit or the χ^2 fit, where e_0 and Δe are two parameters that need to be determined. In Table 1, e_n is a measured data point in units of 10^{-19} Coulomb and σ_{e_n} denotes a standard deviation of each data point. **(30 pts)**

   The following issues should be addressed either in the report.

   (a) Construct χ^2.

   (b) Construct a set of linear equations by minimization of χ^2 with respect to the two unknown parameters.

   (c) Solve the set of linear equations using the Gauss elimination, LU decomposition, or singular value decomposition method (pick one of them and specify which one was used).

   (d) Write down the e_0 and Δe values obtained from the fitting.

   (e) Estimate the standard deviations of the fitting parameter values, and covariance of the two parameters.

   (f) Discuss how good your fit is by calculating the Q value, where $1-Q(\chi^2, \nu) = \gamma(\nu/2, \chi^2/2)/\Gamma(\nu/2)$ and $\nu = N - M$ (degrees of freedom, N is the number of data points and M is the number of parameters). The $\Gamma(a)$ function is simply defined to be $a!$ when the argument a is an integer, and it has the recursion relation $\Gamma(a+1) = a\Gamma(a)$. In the above $\gamma(x, a)$ can be obtained from the series: $\gamma(x, a) = e^{-x}x^a \sum_{n=0}^{\infty} \Gamma(a)x^n/\Gamma(a+1+n)$. The Q value can be computed using this series representation.

   (g) Print out the differences between the data and the values obtained from the model linear function $e_n = ne_0 + \Delta e$ after the fitting. Plot the data with the model function.

   (h) If the standard deviations for the data are not provided, the value of $Q(chi^2, \nu)$ would be meaningless. By setting σ_{e_n}=1, compute χ^2 again and check if the fitted parameter values e_0 and Δe change compared to the previous case.

Table 1: Data from the Millikan experiment

n	5	6	7	8	9	10	11
e_n	8.206	9.880	11.50	13.14	14.82	16.40	18.04
σ_{e_n}	0.012	0.015	0.058	0.025	0.035	0.013	0.010
n	12	13	14	15	16	17	18
e_n	19.68	21.32	22.96	24.60	26.24	27.88	29.52
σ_{e_n}	0.039	0.010	0.019	0.020	0.011	0.030	0.048

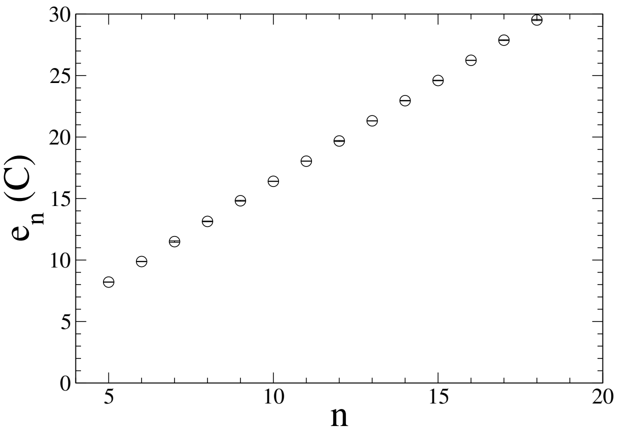

Figure 1: Millikan measurements of charges in oil drop experiments with fictitious error bars.

2. Write a program to fit the following data (shown in Fig.2 and Table 2) to a nonlinear function $y(x; a, k) = ax\exp(-kx)$ by using the Levenberg-Marquardt method. You may start with an initial guess of $a = 3.1$ and $k = 0.4$. **(30 pts)**

   (i) Find the fitting parameters a and k. What is your fudge factor λ? To solve the equations for the update of the parameter values, you may consider using the Gauss elimination method or LU decomposition method with partial *pivoting* or the SVD method. (ii) Find the standard deviations of the parameter values. (iii) Find the covariance of the two parameter values. (iv) Print out the differences between y_i and $y(x_i; a_f, k_f)$, where a_f and k_f are the parameter values obtained from the fitting. (v) Plot the data with the model function $y(x; a_f, k_f) = a_f x\exp(-k_f x)$, where a_k and k_f are the fitting parameter values. (vi) Vary your initial guess of a and k to see if the fitted values of a and k change. (vii) How about changing the initial value of λ (fudge factor)? Would this affect your final answer?

Table 2: 11 data points fitted to the nonlinear model: $y(x; a, k) = ax\exp(-kx)$.

x_i	y_i	σ_y
0	-0.02802838	0.0025
2	6.107835	0.095
4	8.233952	0.086
6	8.526069	0.175
8	7.438678	0.064
10	6.297892	0.045
12	5.045212	0.033
14	3.989115	0.041
16	3.077397	0.053
18	2.355075	0.030
20	1.582216	0.025

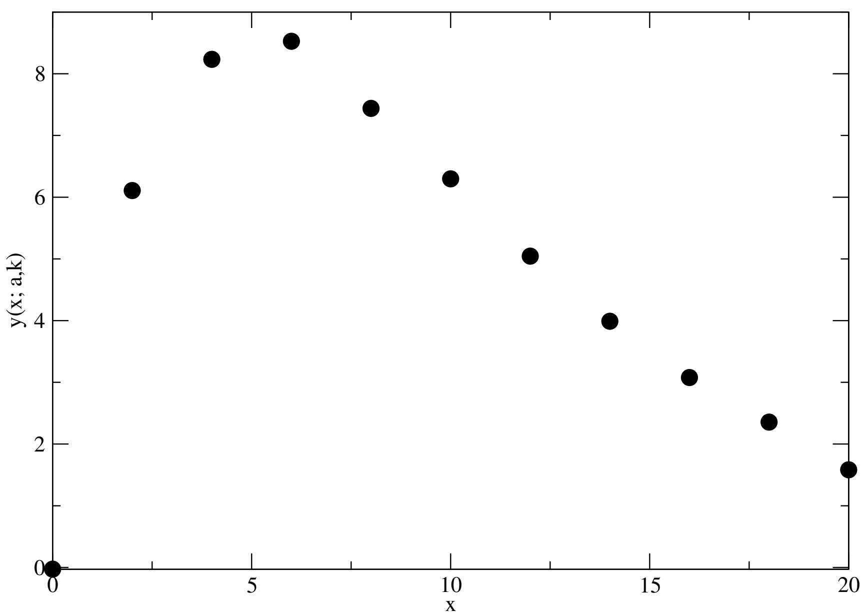

Figure 2: 11 data points shown in Table 2.