Lecture 18

APPLICATION OF PROBABILITY THEORY TO PHYSICAL MEASUREMENTS

Suppose we wish to determine the charge e and mass m of the electron. The Millikan oil-drop experiment measures e directly. The deflection of an electron beam in a known electromagnetic field measures the ratio (e/m). The deflection of an electron beam toward a metal plate due to attraction of image charges measures (e^2/m).

From the results of any two of these experiments we can calculate values of e and m. But all the measurements are subject to error, and the values of e, m obtained from different experiments will not agree. How, then, do we process the data so as to make use of all the information available and get the best estimates of e, m? What is the probable error remaining? How much would the situation be improved by including still another experiment of given accuracy? In this lecture I want to show that probability theory gives simple and elegant answers to these questions.

18.1. Reduction of Equations of Condition.

More specifically, suppose we have the results of these experiments:

(1) measures e with ±2% accuracy

(2) measures (e/m) with ±1% accuracy

(3) measures (e^2/m) with ±5% accuracy

Supposing the values of e, m approximately known in advance, $e \approx e_o$, $m \approx m_o$, the measurements are then linear functions of the corrections. Write the

unknown true values of e and m as

$$e = e_o(1 + x_1)$$
$$m = m_o(1 + x_2) \qquad (18\text{-}1)$$

then x_1, x_2 are dimensionless corrections, small compared to unity, and our problem is to find the best estimate of x_1 and x_2. The results of the three measurements are three numbers M_1, M_2, M_3 which we write as

$$M_1 = e_o(1 + y_1)$$
$$M_2 = \frac{e_o}{m_o}(1 + y_2)$$
$$M_3 = \frac{e_o^2}{m_o}(1 + y_3) \qquad (18\text{-}2)$$

where the y_i are also small dimensionless numbers which are defined by (18-2) and are therefore known in terms of the old estimates e_o, m_o and the new measurements M_1, M_2, M_3. On the other hand, the true values of e, e/m, e^2/m are expressible in terms of the x_i:

$$e = e_o(1 + x_1)$$
$$\frac{e}{m} = \frac{e_o(1 + x_1)}{m_o(1 + x_2)} = \frac{e_o}{m_o}(1 + x_1 - x_2 + \ldots)$$
$$\frac{e^2}{m} = \frac{e_o^2(1 + x_1)^2}{m_o(1 + x_2)} = \frac{e_o^2}{m_o}(1 + 2x_1 - x_2 + \ldots) \qquad (18\text{-}3)$$

where higher order terms are considered negligible. Comparing (18-2) and (18-3) we see that if the measurements were exact we would have

$$y_1 = x_1$$
$$y_2 = x_1 - x_2$$
$$y_3 = 2x_1 - x_2$$

But taking into account the errors, the known y_i are related to the unknown x_j by

$$y_1 = a_{11} x_1 + a_{12} x_2 + \delta_1$$

$$y_2 = a_{21} x_1 + a_{22} x_2 + \delta_2$$

$$y_3 = a_{31} x_1 + a_{32} x_2 + \delta_3 \qquad (18\text{-}4)$$

where the coefficients a_{ij} form a (3 x 2) matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & -1 \\ 2 & -1 \end{pmatrix} \qquad (18\text{-}5)$$

and the δ_i are the unknown fractional errors of the three measurements. For example, the statement $\delta_2 = -0.01$ means that the second measurement gave a result one per cent too small.

More generally, we have n unknown quantities $\{x_1 \ldots x_n\}$ to be estimated from N imperfect observations $\{y_1 \ldots y_N\}$, with $N \geq n$, and the N "equations of condition,"

$$y_i = \sum_{j=1}^{n} a_{ij} x_j + \delta_i \ , \quad i = 1, 2, \ldots, N. \qquad (18\text{-}6)$$

or, in matrix notation,

$$y = Ax + \delta \qquad (18\text{-}7)$$

where A is an (N x n) matrix.

It seems plausible that the best estimate of each x_j will be some linear combination of all the y_i, but if N > n we cannot simply solve equation (18-7) for x, since A is not a square matrix and has no inverse. However, we can get a system of equations solvable for x if we take n linear combinations of the equations of condition; i.e., if we multiply (18-7) on the left by some (n x N) matrix B. Then the product BA exists and is a square (n x n)

matrix. Choose B so that $(BA)^{-1}$ exists. Then the linear combinations are the n rows of

$$By = BAx + B\delta \tag{18-8}$$

which has the unique solution

$$x = (BA)^{-1} B(y - \delta) \tag{18-9}$$

If the probabilities of various fractional errors δ_i are symmetric: $p(\delta_i) = p(-\delta_i)$ so that $\langle\delta_i\rangle = 0$, then corresponding to any given matrix B the "best" estimate of x_j by almost any criterion will be the j'th row of

$$\bar{x} = (BA)^{-1} By \tag{18-10}$$

But by making different choices of B (i.e. taking different linear combinations of the equations of condition) we get different estimates. Which choice of B is best?

In the above I have merely restated, in modern terms, the old problem of "reduction of equations of condition" studied by 18'th century astronomers and described in Laplace's "Essai Philosophique." A popular criterion for solution was the principle of least squares; find that matrix B for which the sum of the squares of the errors in $\bar{x}_j$ is a minimum; or perhaps use a weighted sum. This problem can be solved directly.

18.2. Reformulation as a Decision Problem.

But we really solved this problem in Lecture 13, for we have already shown in full generality that the best estimate of any parameter (or any quantity, if you are squeamish about calling every unknown quantity a "parameter), by the criterion of any loss function, is found by applying Bayes' theorem to find the probability that the parameter lies in various intervals, then making that estimate which minimizes the expected loss taken over the posterior probabilities.

Now in the original formulation of the problem, as given above, it was

only a plausible conjecture that the best estimate of x_j is a linear combination of the y_i as in Equation (18-10). The material in Lecture 13 shows us a much better way of formulating the problem, in which we don't have to depend on conjecture. Instead of trying to take linear combinations without knowing which combinations to take, we should apply Bayes' theorem directly to the equations of condition. Then, if the best estimates are indeed of the form (18-10), Bayes' theorem should not only tell us that fact, it will automatically give us also the best choice of the matrix B.

Let's do this calculation for the case the probabilities assigned to the errors δ_i of the various measurements are independent and gaussian. We expect this to be the most realistic case, since in most physical measurements the total error is the sum of contributions from many small imperfections, and the central limit theorem, to be discussed later, would then lead us to the gaussian form. To anticipate a little, this is subject to one important qualification; that in general the gaussian approximation will be good only for those values of total error δ which can arise in many different ways by combination of the individual elementary errors. For unusually wide deviations the gaussian approximation can be very bad--just how bad we will see later when we study the Cauchy distribution.

The probability that the errors $\{\delta_1 \ldots \delta_N\}$ lie in the intervals $d\delta_1 \ldots d\delta_N$ respectively, is

$$p(\delta_1 \ldots \delta_N)\, d\delta_1 \ldots d\delta_N = (\text{const.})\, \exp\left[-\frac{1}{2} \sum_{i=1}^{N} w_i \delta_i^{\,2} \right] d\delta_1 \ldots d\delta_N \qquad (18\text{-}11)$$

where the "weight" w_i is the reciprocal variance of the error of the i'th measurement. For example, the crude statement that the first measurement has ±2 per cent accuracy, now becomes the more precise statement that the first measurement has weight

$$w_1 = \frac{1}{\langle \delta_1^{\,2} \rangle} = \frac{1}{(.02)^2} = 2500 \qquad (18\text{-}12)$$

From (18-6) and (18-11) we have immediately the probability density for obtaining measured values $\{y_1 \ldots y_N\}$ given the true values $\{x_1 \ldots x_n\}$:

$$(y_1 \ldots y_N | x_1 \ldots x_n) = C_1 \exp\left\{ -\frac{1}{2} \sum_{i=1}^{N} w_i [y_i - \sum_{j=1}^{n} \alpha_{ij} x_j]^2 \right\} \quad (18\text{-}13)$$

where C_1 is independent of the y_i. According to Bayes' theorem, if we assign uniform prior probabilities to the x_j, then the posterior probability density for the x_j, given the actual measurements y_i, is of the form

$$(x_1 \ldots x_n | y_1 \ldots y_N) = C_2 \exp\left\{ -\frac{1}{2} \sum_{i=1}^{N} w_i [y_i - \sum_{j=1}^{n} a_{ij} x_j]^2 \right\} \quad (18\text{-}14)$$

where C_2 is independent of the x_j. Now

$$\sum_{i=1}^{N} w_i (y_i - \sum_{j=1}^{n} a_{ij} x_j)^2$$

$$= \sum_{i=1}^{N} w_i [y_i^2 - 2y_i \sum_{j=1}^{n} a_{ij} x_j + \sum_{j,k=1}^{n} a_{ij} a_{ik} x_j x_k]$$

$$= \sum_{j,k=1}^{n} K_{jk} x_i x_k - 2 \sum_{j=1}^{n} L_j x_j + \sum_{i=1}^{N} w_i y_i^2 \quad (18\text{-}15)$$

where

$$K_{jk} \equiv \sum_{i=1}^{N} w_i a_{ij} a_{ik} \quad (18\text{-}16)$$

$$L_j \equiv \sum_{i=1}^{N} w_i y_i a_{ij} \quad (18\text{-}17)$$

or, defining a diagonal "weight" matrix $W_{ij} = w_i \delta_{ij}$, we have a matrix K and a vector L:

$$K = \tilde{A} W A \quad (18\text{-}18)$$

$$L = \tilde{A} W y \quad (18\text{-}19)$$

where $\tilde{A}$ is the transposed matrix. We want to write (18-14) in the form

$$(x_1 \ldots x_n | y_1 \ldots y_N) = C_3 \exp[-\frac{1}{2} \sum_{j,k=1}^{n} K_{jk} (x_j - \bar{x}_j)(x_k - \bar{x}_k)] \quad (18\text{-}20)$$

whereupon the $\bar{x}_j$ will be the mean value estimates desired. Comparing (18-15) and (18-20) we see that

$$\sum_{k=1}^{n} K_{jk} \bar{x}_k = L_j \quad (18\text{-}21)$$

or,

$$\bar{x}_k = \sum_{j=1}^{n} (K^{-1})_{kj} L_j \tag{18-22}$$

and this is the solution for best estimates of the $\bar{x}_k$ by the mean-square error criterion. From (18-18) and (18-19), we can write the result as

$$\bar{x} = (\tilde{A} W A)^{-1} \tilde{A} W y \tag{18-23}$$

and, comparing with (18-10), we see that in the gaussian case with uniform prior probabilities, the best estimates are indeed of the form (18-10), and the best choice of the matrix B is

$$B = \tilde{A} W \quad , \tag{18-24}$$

a result given by Laplace (1819).

Let us apply this solution to our determination of e and m. Here the measurements of e, (e/m), (e^2/m) were of 2%, 1%, 5% accuracy respectively, and so

$$w_2 = \frac{1}{(.01)^2} = 10{,}000$$

$$w_3 = \frac{1}{(.05)^2} = 400 \tag{18-25}$$

and we found $w_1 = 2500$ before. Thus we have

$$B = \tilde{A} W = \begin{pmatrix} 1 & 1 & 2 \\ 0 & -1 & -1 \end{pmatrix} \begin{pmatrix} w_1 & 0 & 0 \\ 0 & w_2 & 0 \\ 0 & 0 & w_3 \end{pmatrix} = \begin{pmatrix} w_1 & w_2 & 2w_3 \\ 0 & -w_2 & -w_3 \end{pmatrix} \tag{18-26}$$

$$K = \tilde{A} W A = \begin{pmatrix} (w_1+w_2+4w_3) & -(w_2+2w_3) \\ -(w_2+2w_3) & (w_2+w_3) \end{pmatrix} \tag{18-27}$$

$$K^{-1} = (\tilde{A} W A)^{-1} = \frac{1}{\Delta} \begin{pmatrix} (w_2+w_3) & (w_2+2w_3) \\ (w_2+2w_3) & (w_1+w_2+4w_3) \end{pmatrix} \tag{18-28}$$

where

$$\Delta = \det(K) = w_1w_2 + w_2w_3 + w_3w_1 \tag{18-29}$$

Thus the final result is

$$(\tilde{A}\ W\ A)^{-1}\ \tilde{A}\ W = \frac{1}{\Delta}\begin{pmatrix} w_1(w_2+w_3) & -w_2w_3 & w_2w_3 \\ w_1(w_2+2w_3) & -w_2(w_1+2w_3) & w_3(w_2-w_1) \end{pmatrix} \tag{18-30}$$

and the best estimates of x_1, x_2 are

$$\bar{x}_1 = \frac{w_1(w_2+w_3)y_1 + w_2w_3(y_3-y_2)}{w_1w_2 + w_2w_3 + w_3w_1} \tag{18-31}$$

$$\bar{x}_2 = \frac{w_1w_2(y_1-y_2) + w_2w_3(y_3-2y_2) + w_3w_1(2y_1-y_3)}{w_1w_2 + w_2w_3 + w_3w_1} \tag{18-32}$$

Inserting the numerical values of w_1, w_2, w_3, we have

$$\bar{x}_1 = \frac{13}{15}\,y_1 + \frac{2}{15}\,(y_2-y_3) \tag{18-33}$$

$$\bar{x}_2 = \frac{5}{6}\,(y_1-y_2) + \frac{2}{15}\,(y_3-2y_2) + \frac{1}{30}\,(2y_1-y_3) \tag{18-34}$$

which exhibits the best estimates as weighted averages of the estimates taken from all possible pairs of experiments. Thus, y_1 is the estimate of x_1 obtained in the first experiment, which measures e directly. The second and third experiments combined give an estimate of e given by $(e^2/m)(e/m)^{-1}$. Since

$$\frac{\frac{e_o^2}{m_o}(1+y_3)}{\frac{e_o}{m_o}(1+y_2)} \simeq e_o(1+y_3-y_2)$$

(y_3-y_2) is the estimate of x_1 given by experiments 2 and 3. Equation (18-33) says that these two independent estimates of x_1 should be combined with weights 13/15, 2/15. Likewise, Equation (18-34) gives $\bar{x}_2$ as a weighted average of three different (although not independent) estimates of x_2.

But how accurate are these estimates $\bar{x}_j$? From (18-20) we find the well-known formula for the second central moments of $(x_1 \ldots x_n | y_1 \ldots y_N)$:

$$\langle \Delta x_j \Delta x_k \rangle \equiv \langle (x_j - \bar{x}_j)(x_k - \bar{x}_k) \rangle = \langle x_j x_k \rangle - \langle x_j \rangle \langle x_k \rangle = (K^{-1})_{jk} \qquad (18\text{-}35)$$

Thus from the inverse matrix

$$K^{-1} = (\tilde{A}\, W\, A)^{-1} \qquad (18\text{-}36)$$

already found in our calculation of $\bar{x}_j$, we can also read off the probable errors, or more conveniently, the standard deviations. From (18-27) we can state the results in the form (mean) ± (standard deviation) as

$$x_j = \bar{x}_j \pm \sqrt{(K^{-1})_{ij}} \qquad (18\text{-}37)$$

or,

$$x_1 = \bar{x}_1 \pm \left[\frac{w_2 + w_3}{w_1 w_2 + w_2 w_3 + w_3 w_1} \right]^{1/2} \qquad (18\text{-}38)$$

$$x_2 = \bar{x}_2 \pm \left[\frac{w_1 + w_2 + 4w_3}{w_1 w_2 + w_2 w_3 + w_3 w_1} \right]^{1/2} \qquad (18\text{-}39)$$

with numerical values

$$x_1 = \bar{x}_1 \pm 0.0186$$
$$x_2 = \bar{x}_2 \pm 0.0216 \qquad (18\ 40)$$

so that from the three measurements we obtain e with ±1.86 per cent accuracy, m with ±2.16 per cent accuracy.

How much did the rather poor measurement of (e^2/m), with only ±5 per cent accuracy, help us? To answer this, note that in the absence of this experiment we would have arrived at conclusions given by (18-27), (18-31) and (18-32) in the limit $w_3 \to 0$. The results (also easily verified directly from the statement of the problem) are

$$\bar{x}_1 = y_1$$
$$\bar{x}_2 = y_1 - y_2 \qquad (18\text{-}41)$$

$$K^{-1} = \frac{1}{w_1 w_2}\begin{pmatrix} w_2 & w_2 \\ w_2 & (w_1+w_2) \end{pmatrix} \tag{18-42}$$

or, the (mean) ± (standard deviation) values are

$$x_1 = y_1 \pm \frac{1}{\sqrt{w_1}} = y_1 \pm 0.020$$

$$x_2 = y_1 - y_2 \pm \left[\frac{w_1+w_2}{w_1 w_2}\right]^{1/2} = y_1 - y_2 \pm 0.024 \tag{18-43}$$

As might have been anticipated by common sense, a low-accuracy measurement can add very little to the results of accurate measurements, and if the (e^2/m) measurement had been much worse than ±5 per cent it would hardly be worth-while to include it in our calculations. But suppose that an improved technique gives us an (e^2/m) measurement of ±2 per cent accuracy. How much would this help? The answer is given by our previous formulas with $w_1 = w_3 = 2500$, $w_2 = 10{,}000$. We find now that the mean-value estimates give much higher weight to the estimates using the (e^2/m)) measurement:

$$\bar{x}_1 = 0.556\, y_1 + 0.444(y_3 - y_2)$$

$$\bar{x}_2 = 0.444(y_1 - y_2) + 0.444(y_3 - 2y_2) + 0.112(2y_1 - y_3) \tag{18-44}$$

which is to be compared with (18-33), (18-34). The standard deviations are given by

$$x_1 = \bar{x}_1 \pm 0.0149$$

$$x_2 = \bar{x}_2 \pm 0.020 \tag{18-45}$$

The accuracy of e is improved roughly twice as much as that of m, since the improved measurement involves e^2, but only the first power of m.

18.3. Discussion: A Paradox.

We can learn many more things from studying this problem. For example,

I want to point out something which you will find astonishing at first. If you study Equation (18-32), which gives the best estimate of m from the three measurements, you will see that y_3, the result of the (e^2/m) measurement, enters into the formula in a different way than y_1 and y_2. It appears once with a positive coefficient, and once with a negative one. If $w_1 = w_2$, these coefficients are equal and (18-32) collapses to

$$\overline{x}_2 = y_1 - y_2 \qquad (18\text{-}46)$$

Now, realize the full implications of this: it says that the only reason we make use of the (e^2/m) measurement in estimating m is that the (e) measurement and the (e/m) measurement have different accuracy. No matter how accurately we know (e^2/m), if the (e) and (e/m) measurements happen to have the same accuracy, however poor, then we should ignore the good measurement and base our estimate of m only on the (e) and (e/m) measurements!

I think that your common sense will instantly revolt against this conclusion, and you will say that there must be an error in Equation(18-32). So, let's take a minute off while you check the derivation.

This is a perfect example of the kind of result which probability theory gives us almost without effort, but which our unaided common sense might not notice in years of thinking about the problem. I won't deprive you of the pleasure of resolving this "paradox" for yourself, and explaining to your friends how it can happen that consistent inductive reasoning may demand that you throw away your best measurement.

You recall that, back at the end of Lecture 9, I complained about the fact that orthodox statisticians sometimes throw away relevant data in order to fit a problem to their model of "independent random errors." Am I now guilty of advocating the same thing? No doubt, it looks very much that way! Yet I plead innocence--the numerical value of (e^2/m) is in fact irrelevant to inference about m, if we already have measurements of e and e/m of equal

accuracy. Try drawing diagrams--or just try and figure out how you would use (e^2/m) in this situation--and I think you'll see why this is so.

As another example, it is important that we understand the way our conclusions depend on our choice of loss functions and probability distributions for the errors δ_i. If we use instead of the Gaussian distribution (18-11) one with wider tails, such as the Cauchy distribution $p(\delta) \propto (1 + \frac{1}{2}w\delta^2)^{-1}$, the posterior distribution $(x_1x_2|y_1y_2y_3)$ may have more than one peak in the (x_1,x_2)-plane. Then a quadratic loss function, or more generally any concave loss function (i.e. doubling the error more than doubles the loss) will lead you to make estimates of x_1 and x_2 which lie between the peaks, and are known to be very unlikely. With a convex loss function a different "paradox" appears, in that the basic equation (13-16) for constructing the best estimator may have more than one solution, with nothing to tell us which one to use.

The appearance of these situations is the robot's way of telling us this: our state of knowledge about x_1 and x_2 is too complicated to be described adequately simply by giving estimates and probable errors. The only honest way of describing what we know is to give the actual distribution $(x_1x_2|y_1y_2y_3)$. This is one of the limitations of decision theory which we have to understand in order to use it properly.