Chapter 8 Approximation Theory

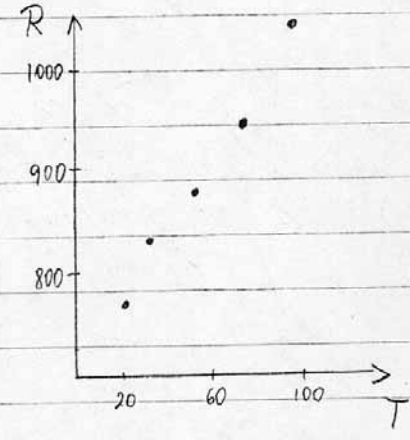
8.1 Discrete Least Squares Approximation

Until now we have assumed that data are accurate, but when these values are derived from an experiment, there is some error in the measurements. This section introduces the usual method of treating such data.

1) Approximating with a line

Ex. Suppose one wants to find the effect of temperature on the resistance of a metal wire. Suppose the following data are recorded

T, °C	R, ohms
20.5	765
32.7	826
51.0	873
73.2	942
95.7	1032



From these data it looks that the relationship between the temperature and the resistance is linear

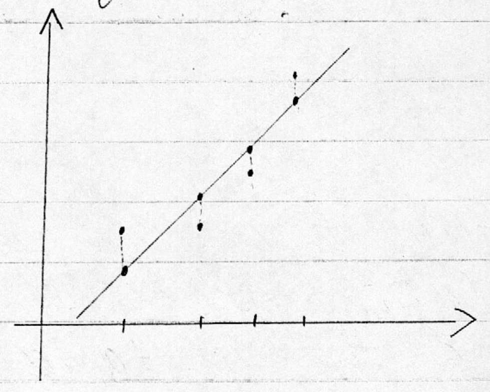
$R = aT + b$

But no line can go through all the points because there is error in them.

It is unreasonable to interpolate these data since the interpolating polynomial will be with a high degree with oscillations which are not originally present.

There are many ways to draw a line through these data. We want the "best" in some sense line.

We define the best line as the line for which the sum of the squares of the differences between the y-values of the point on the line and the given y-value is as small as possible.



The method used to obtain this line is called <u>least-squares method</u>.

To explain the method, let Y_i be the y-coordinates of the experimental data and let

$$y_i = ax_i + b \qquad i = 1, .., n$$

where x_i is the value of the variable assumed to be free of error.

The differences of the y-coordinates are

$$Y_i - y_i \qquad i = 1, .., n$$

or

$$Y_i - ax_i - b$$

So we square them and add them to get

$$E = E(a, b) = \sum_{i=1}^{n} (Y_i - ax_i - b)^2$$

We want to find $a, b = ?$ so that E is as small as possible. For a minimum to occur we need

$$\frac{\partial E}{\partial a} = 0 \qquad \frac{\partial E}{\partial b} = 0$$

$$\frac{\partial E}{\partial a} = \sum_{i=1}^{n} 2(Y_i - a x_i - b)(-x_i) = 0$$

$$\frac{\partial E}{\partial b} = \sum_{i=1}^{n} 2(Y_i - a x_i - b)(-1) = 0$$

This simplifies to the following system of normal equations

$$a\left(\sum_{i=1}^{n} x_i^2\right) + b\left(\sum_{i=1}^{n} x_i\right) = \sum_{i=1}^{n} Y_i x_i$$
$$a\left(\sum_{i=1}^{n} x_i\right) + b \cdot n = \sum_{i=1}^{n} Y_i$$

This is a 2×2 system for a, b which has to be solved.

$$Q_{11}\, a + Q_{12}\, b = R_1$$
$$Q_{12}\, a + Q_{22}\, b = R_2$$

where $Q_{11} = \sum_{i=1}^{n} x_i^2$ $\quad Q_{12} = \sum_{i=1}^{n} x_i$

$Q_{22} = n \quad R_1 = \sum_{i=1}^{n} Y_i x_i \quad R_2 = \sum_{i=1}^{n} Y_i$

The solution is

$$a = \frac{nR_1 - Q_{12}R_2}{nQ_{11} - Q_{12}^2}$$

$$b = \frac{Q_{11}R_2 - R_1 Q_{12}}{nQ_{11} - Q_{12}^2}$$

Ex: Find the least square polynomial
#3/494 of degree 1 for the data in the following table. Compute the error E

x_i	1.0	1.1	1.3	1.5	1.9	2.1
y_i	1.84	1.96	2.21	2.45	2.94	3.18

We do that in the following expanded table

	x_i	y_i	x_i^2	$x_i y_i$	$ax_i + b$	$(y_i - ax_i - b)^2$
1	1.0	1.84	1.0	1.84	1.84051634	$2.666 \cdot 10^{-7}$
2	1.1	1.96	1.21	2.156	1.96247847	$6.1428 \cdot 10^{-6}$
3	1.3	2.21	1.69	2.873	2.2064	$1.296 \cdot 10^{-5}$
4	1.5	2.45	2.25	3.675	2.450327	$1.06929 \cdot 10^{-7}$
5	1.9	2.94	3.61	5.586	2.93817555	$3.32861 \cdot 10^{-6}$
6	2.1	3.18	4.41	6.678	3.1821	$4.4 \cdot 10^{-6}$
	8.9	14.58	14.17	22.808		$2.72 \cdot 10^{-5}$
	Q_{12}	R_2	Q_{11}	R_1		↑ error

Substituting in the formulas for a, b we have

$$a = \frac{6\cdot(22.808) - (8.9)(14.58)}{6\cdot(14.17) - (8.9)^2} = \frac{7.086}{5.81}$$

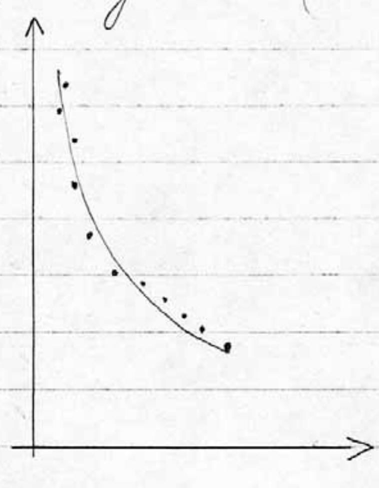
$$a = 1.219621343$$

$$b = \frac{(14.17)(14.58) - (22.808)(8.9)}{6(14.17) - (8.9)^2} = \frac{3.6074}{5.81}$$

$$b = 0.620895$$

2) Approximating with a quadratic

Sometimes the data are not best fitted by a line or we just want to approximate them by a polynomial of degree 2 (or higher)



So suppose we want to fit a quadratic

$$y = ax^2 + bx + c$$

through the points (x_i, Y_i) $i = 1, \ldots, n$.

Thus, the points on the quadratic with x_i coordinates are

$$y_i = ax_i^2 + bx_i + c$$

The distances between the approximat. y-values and y_i are

$$Y_i - y_i$$

Thus, the error is

$$E = E(a, b, c) = \sum_{i=1}^{n} (Y_i - ax_i^2 - bx_i - c)^2$$

The minimum is attained when

$$\frac{\partial E}{\partial a} = \sum_{i=1}^{n} 2(Y_i - ax_i^2 - bx_i - c)(-x_i^2) = 0$$

$$\frac{\partial E}{\partial b} = \sum_{i=1}^{n} 2(Y_i - ax_i^2 - bx_i - c)(-x_i) = 0$$

$$\frac{\partial E}{\partial c} = \sum_{i=1}^{n} 2(Y_i - ax_i^2 - bx_i - c)(-1) = 0$$

Rearranging these equations, we can obtain the normal equations

Rearranging this system we obtain the system of normal equations

$$a\left(\sum x_i^4\right) + b\left(\sum x_i^3\right) + c\left(\sum x_i^2\right) = \sum Y_i x_i^2$$

$$a\left(\sum x_i^3\right) + b\left(\sum x_i^2\right) + c\left(\sum x_i\right) = \sum Y_i x_i$$

$$a\left(\sum x_i^2\right) + b\left(\sum x_i\right) + c \cdot n \quad = \sum Y_i$$

which has to be solved for a, b, c.

Notice: the matrix of coefficients is symmetric.

Ex. Use least-squares and a second degree polynomial to fit the data

x_i	0.05	0.11	0.15	0.31	0.46	0.52
Y_i	0.956	0.89	0.832	0.717	0.571	0.539

x_i	0.70	0.74	0.82	0.98	1.171
Y_i	0.378	0.37	0.306	0.242	0.104

	x_i	Y_i	x_i^2	x_i^3	x_i^4	$Y_i x_i$	$Y_i x_i^2$
	0.05	0.956	0.0025	0.000125	0.00000625	0.0478	0.023
	0.11	0.89	0.0121	0.001331	0.00014641	0.0979	0.010
	0.15	0.832	0.0225	0.003375	0.00050625	0.1248	0.018
	0.31	0.717	0.0961	0.029791	0.00923521	0.22227	0.068
	0.46	0.571	0.2116	0.097336	0.0447746	0.26266	0.1208
	0.52	0.539	0.2704	0.140608	0.07311616	0.28028	0.145
$n = 11$	0.72	0.378	0.5184	0.373248	0.2687385	0.27216	0.195
	0.74	0.37	0.5476	0.405224	0.299866	0.2738	0.202
	0.82	0.306	0.6724	0.551368	0.452122	0.25092	0.205
	0.98	0.242	0.9604	0.941192	0.92237	0.23716	0.232
	1.171	0.104	1.371241	1.6057	1.8803	0.121784	0.142
	6.01	5.905	4.6545	4.1150	3.9161	2.1839	1.335

Thus, we get the following system of normal equations

$$3.9161\,a + 4.115\,b + 4.6545\,c = 1.3357$$
$$4.115\,a + 4.6545\,b + 6.01\,c = 2.1839$$
$$4.6545\,a + 6.01\,b + 11\,c = 5.905$$

The solution to this system is

$$a = 0.225 \quad b = -1.018 \quad c = 0.998$$

Thus:

$$P(x) = 0.225x^2 - 1.018x + 0.998$$

3) Fitting other types of curves.

In many cases the data are not linear and we might want to fit some function other than a polynomial. Popular forms are

$$y = f(x) = be^{ax}$$

or

$$y = g(x) = bx^{a}$$

In this case the system of normal equations is NOT linear and is often difficult to solve. One approach to deal with the problem is to take ln of both sides

$$\ln y = \ln b + ax$$

or

$$\ln y = \ln b + a\ln x$$

If we set $z = \ln y$, $B = \ln B$ these equations become

$$z = B + ax$$

$$z = B + a \cdot \ln x$$

Thus, we fit a new variable z to x (or $\ln x$). In each case the relationship is linear.

Ex. These data measure the solubilities of n-butane in liquid anhydrous hydro-flouric acid.

$T, {}^\circ F$	77	100	185	239	285
S, wt.%	2.4	3.4	7.0	1.1	19.6

Fit these data to the equation

$$S = a e^{bT}$$

Solution: Consider

$$\ln S = \ln a + bT$$

or:

$$y = A + bT$$

T_i	S_i	$\ln S_i$ (Y_i)	T_i^2	$T_i \ln S_i$
77	2.4	0.875469	5929	67.411
100	3.4	1.223775	10000	122.3775
185	7.0	1.94591	34225	359.99
239	1.1	0.09531	57121	22.779
285	19.6	2.97553	81225	848.0259
886		7.115994	188500	1420.5834

The normal equations are

$$b\left(\sum_i' T_i^2\right) + A\left(\sum_i' T_i\right) = \sum_i' T_i \ln S_i$$

$$b\left(\sum_i' T_i\right) + A \cdot 5 = \sum' \ln S_i$$

or explictly:

$$188500\, b + 886\, A = 1420.5834$$
$$886\, b + 5\, A = 7.115994$$

Thus

$$b = \frac{5 \cdot (1420.5834) - 886\,(7.115994)}{5 \cdot 188500 - (886)^2} = \frac{798.146}{157504}$$

$$b = 0.0050675$$

$$A = \frac{188500\,(7.115994) - (1420.5834)(886)}{5 \cdot 188500 - (886)^2}$$

$$A = 0.52524$$

Since $\ln a = A \Rightarrow \ln a = 0.52524$

$$a = e^{0.52524}$$
$$a = 1.69$$

Thus:

$$S = 1.69\, e^{0.0050675\, T}$$