Least Squares Method and Orthogonal Systems

Section 9.1 and 9.2

CS 3010

Numerical Methods

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Linear Least Squares Method

- Data produced from most experiments in this form (m+1 data points)

x	x_0	x_1	$\cdots$	x_m
y	y_0	y_1	$\cdots$	y_m

- A reasonable tentative conclusion is that the underlying function is *linear* and that the failure of the points to fall *precisely* on a straight line is due to experimental error
- How to determine the correct linear function?

$$y = ax + b$$

- So, what are the coefficients *a* and *b* ?
- What line most nearly passes through the *m+1 points* plotted?

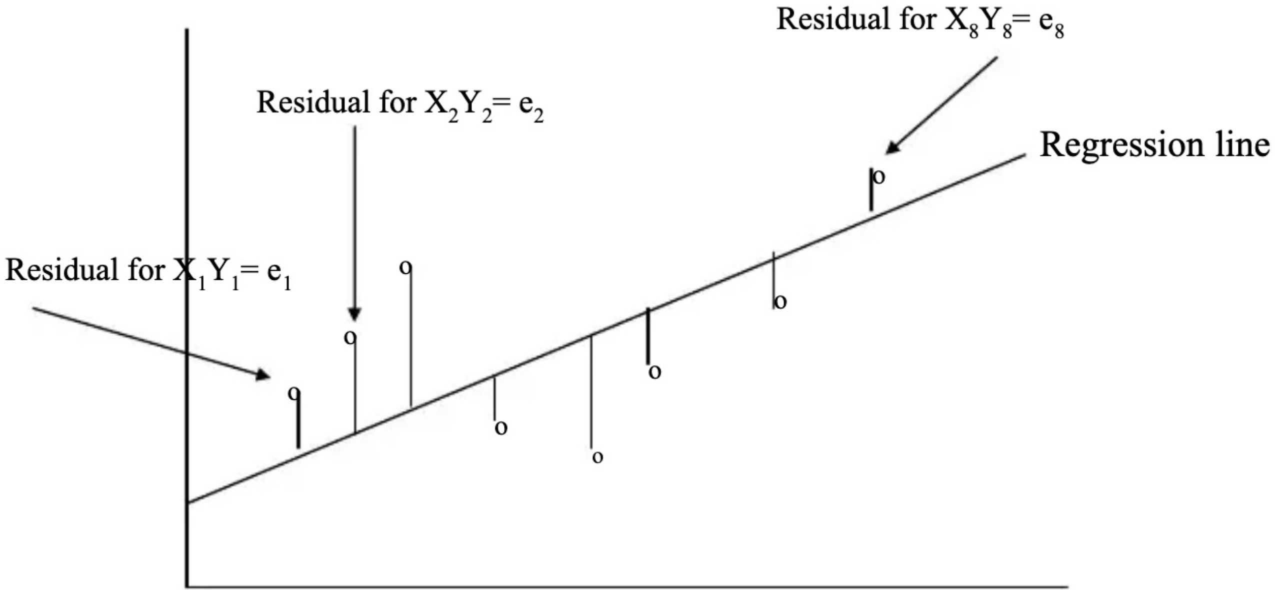
Linear Least Squares Method

- In general, all data points may not fall on the line y = $ax + b$
- If say the kth point falls on the line, then $ax_k + b - y_k = 0$
- If it does not, then there is a discrepancy or *error* of magnitude e_k

$$e_k = |ax_k + b - y_k|$$

- The total absolute error for all $m + 1$ points is therefore

$$e_k = \sum_{k=0}^{m} |ax_k + b - y_k|$$



Linear Least Squares Method

- This is a function of *a* and *b*, and it would be reasonable to choose *a* and *b* so that the function assumes its minimum value.

$$e_k = \sum_{k=0}^{m} |a x_k + b - y_k|$$

- This problem is an example of l_1 **approximation** and can be solved by the techniques of linear programming (beyond the scope of this class)
- it is common to minimize a different error function of *a* and *b*. *i.e. the* l_2 **approximation (**advantage is that the methods of calculus can be used)

$$\varphi(a, b) = \sum_{k=0}^{m} (a x_k + b - y_k)^2$$

- Make $\varphi(a, b)$ a minimum ⇒ By calculus, the conditions

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

Linear Least Squares Method

- Taking Derivatives wrt *a* and *b*, one gets

$$\begin{cases} \displaystyle\sum_{k=0}^{m} 2(ax_k + b - y_k)x_k = 0 \\ \displaystyle\sum_{k=0}^{m} 2(ax_k + b - y_k) = 0 \end{cases}$$

- This is a pair of simultaneous linear equations in the unknowns *a* and *b*. They are called the **normal equations** and can be written as

$$\begin{cases} \left(\displaystyle\sum_{k=0}^{m} x_k^2\right) a + \left(\displaystyle\sum_{k=0}^{m} x_k\right) b = \displaystyle\sum_{k=0}^{m} y_k x_k \\ \left(\displaystyle\sum_{k=0}^{m} x_k\right) a + \quad (m+1) b = \displaystyle\sum_{k=0}^{m} y_k \end{cases}$$

$\sum_{k=0}^{m} 1 = m + 1$

- To simplify calculations,

$$p = \sum_{k=0}^{n} x_k \qquad q = \sum_{k=0}^{n} y_k \qquad r = \sum_{k=0}^{n} x_k y_k \qquad s = \sum_{k=0}^{n} x_k^2$$

Linear Least Squares Method

- Use Cramer's rule to solve it as its only a 2x2 system of linear equations

$$d = \operatorname{Det}\begin{bmatrix} s & p \\ p & m+1 \end{bmatrix} = (m+1)s - p^2 = (m+1)\left(\sum_{k=0}^{m} x_k^2\right) - \left(\sum_{k=0}^{m} x_k\right)^2$$

$$a = \frac{1}{d}\operatorname{Det}\begin{bmatrix} r & p \\ q & m+1 \end{bmatrix} = \frac{1}{d}\left[(m+1)r - pq\right]$$

$$b = \frac{1}{d}\operatorname{Det}\begin{bmatrix} s & r \\ p & q \end{bmatrix} = \frac{1}{d}\left[sq - pr\right]$$

$$\Rightarrow$$

$$a = \frac{1}{d}\left[(m+1)\left(\sum_{k=0}^{m} x_k y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} y_k\right)\right]$$

$$b = \frac{1}{d}\left[\left(\sum_{k=0}^{m} x_k^2\right)\left(\sum_{k=0}^{m} y_k\right) - \left(\sum_{k=0}^{m} x_k\right)\left(\sum_{k=0}^{m} x_k y_k\right)\right]$$

Linear Least Squares Algorithm

The coefficients in the least-squares line $y = ax + b$ through the set of $m + 1$ data points (x_k, y_k) for $k = 0, 1, 2, \ldots, m$ are computed (in order) as follows:

1. $p = \sum_{k=0}^{m} x_k$

2. $q = \sum_{k=0}^{m} y_k$

3. $r = \sum_{k=0}^{m} x_k y_k$

4. $s = \sum_{k=0}^{m} x_k^2$

5. $d = (m + 1)s - p^2$

6. $a = [(m + 1)r - pq]/d$

7. $b = [sq - pr]/d$

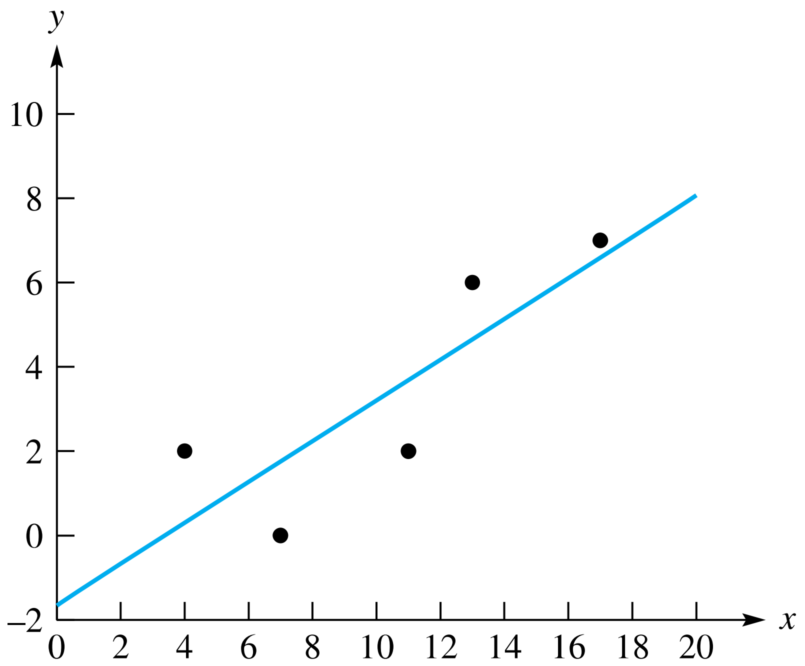
Linear Least Squares Example

x	4	7	11	13	17
y	2	0	2	6	7

- What are the two linear equations if you follow the algorithm?

$$\begin{cases} 644a + 52b = 227 \\ 52a + 5b = 17 \end{cases}$$

$$a = 0.4864 \text{ and } b = -1.6589.$$



Polynomial Least Squares Method

- Let's say we use a quadratic polynomial y = $ax^2 + bx + c$
- Residual error for k^{th} point $e_k = \sum_{k=0}^{m} \left| a x_k^2 + b x_k + c - y_k \right|$
- Error function to minimize is

$$\varphi(a,b,c) = \sum_{k=0}^{m} \left(a x_k^2 + b x_k + c - y_k \right)^2$$

- Taking Derivatives wrt *a, b* and *c*, one gets these three equations

$$\sum_{k=0}^{m} 2\left(a x_k^2 + b x_k + c - y_k \right) x_k^2 = 0$$

$$\sum_{k=0}^{m} 2\left(a x_k^2 + b x_k + c - y_k \right) x_k = 0$$

$$\sum_{k=0}^{m} 2\left(a x_k^2 + b x_k + c - y_k \right) = 0$$

Polynomial Least Squares Method

- Simplifying the equations, one gets a system of linear equations in *a*, *b* and *c,* that can be solved easily to get the quadratic polynomial

$$\left(\sum_{k=0}^{m} x_k^4\right)a + \left(\sum_{k=0}^{m} x_k^3\right)b + \left(\sum_{k=0}^{m} x_k^2\right)c = \sum_{k=0}^{m} y_k x_k^2$$

$$\left(\sum_{k=0}^{m} x_k^3\right)a + \left(\sum_{k=0}^{m} x_k^2\right)b + \left(\sum_{k=0}^{m} x_k\right)c = \sum_{k=0}^{m} y_k x_k$$

$$\left(\sum_{k=0}^{m} x_k^2\right)a + \left(\sum_{k=0}^{m} x_k\right)b + \left(\sum_{k=0}^{m} 1\right)c = \sum_{k=0}^{m} y_k$$

$\sum_{k=0}^{m} 1 = m + 1$

Polynomial Least Squares Method Example

- Find a quadratic polynomial that fits these points

x	-2	-1	0	1	2
y	2	1	1	1	2

$$\sum_{k=0}^{4} 1 = 5 \quad \sum_{k=0}^{4} x_k = 0 \quad \sum_{k=0}^{4} x_k^2 = 10 \quad \sum_{k=0}^{4} x_k^3 = 0 \quad \sum_{k=0}^{4} x_k^4 = 34 \quad \sum_{k=0}^{4} y_k = 7 \quad \sum_{k=0}^{4} y_k x_k = 0 \quad \sum_{k=0}^{4} y_k x_k^2 = 18$$

- Equations to solve are

$5a + 0 + 10c = 7$

$0 + 10b + 0 = 0$

$10a + 0 + 34c = 18$

$a = 29/35$

$b = 0$

$c = 2/7$

$$y = \frac{29}{35} + 0x + \frac{2}{7}x^2 = \frac{29}{35} + \frac{2}{7}x^2$$

Non-Polynomial Non-Linear Least Squares Method

- Let's say functional form to fit is $y = alnx + bcosx + ce^x$
- 3 unknown coefficients

$$\varphi(a,b,c) = \sum_{k=0}^{m} (alnx_k + bcosx_k + ce^{x_k} - y_k)^2$$

- Set $\partial\varphi/\partial a = 0, \partial\varphi/\partial b = 0, \partial\varphi/\partial c = 0$ resulting in

$$\begin{cases} a\sum_{k=0}^{m}(\ln x_k)^2 + b\sum_{k=0}^{m}(\ln x_k)(\cos x_k) + c\sum_{k=0}^{m}(\ln x_k)e^{x_k} = \sum_{k=0}^{m} y_k \ln x_k \\ a\sum_{k=0}^{m}(\ln x_k)(\cos x_k) + b\sum_{k=0}^{m}(\cos x_k)^2 + c\sum_{k=0}^{m}(\cos x_k)e^{x_k} = \sum_{k=0}^{m} y_k \cos x_k \\ a\sum_{k=0}^{m}(\ln x_k)e^{x_k} + b\sum_{k=0}^{m}(\cos x_k)e^{x_k} + c\sum_{k=0}^{m}(e^{x_k})^2 = \sum_{k=0}^{m} y_k e^{x_k} \end{cases}$$

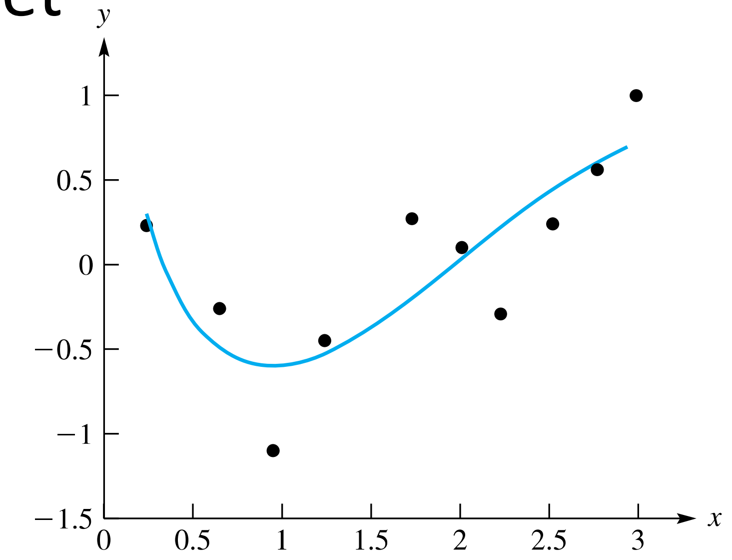
Nonpolynomial Least Square Example

- Fit a function of the form $y = a\ln x + b\cos x + ce^x$ to the following table values:

x	0.24	0.65	0.95	1.24	1.73	2.01	2.23	2.52	2.77	2.99
y	0.23	−0.26	−1.10	−0.45	0.27	0.10	−0.29	0.24	0.56	1.00

- Using the table and equations in the last slide, we get

$$\begin{cases} 6.79410a - 5.34749b + 63.25889c = 1.61627 \\ -5.34749a + 5.10842b - 49.00859c = -2.38271 \\ 63.25889a - 49.00859b + 1002.50650c = 26.77277 \end{cases}$$



- It has the solution $a = -1.04103$, $b = -1.26132$, and $c = 0.03073$.
- Hence, $y = -1.04103 \ln x - 1.26132 \cos x + 0.03073e^x$