Least Squares Method

We are considering $\boldsymbol{M}$ – a set of functions $f(x)$ given as a table in N – points (not necessarily different) and $P \equiv \prod_n(x)$ – polynomials of the *n*-th exponent of variable x. We will regard $\boldsymbol{n} \ll \boldsymbol{N}$. As a measure of the proximity between the function $f(x)$ from set M and $P(x) \in \prod_n(x)$ we will utilize the values of the following function:

$$\Phi(a_0,...,a_n) = \sum_{i=1}^{N}[y_i - (a_n x_i^n + a_{n-1}x_i^{n-1} + ... + a_1 x_i + a_0)]^2,$$

where $a_0,...,a_n$ are the coefficients of the polynomial $P(x)$, a $y_i = f(x_i)$. The polynomial P^*, which has coefficients $a_0^*,...,a_n^*$ minimize the function $\Phi(a_0,...,a_n)$, is called polynomial with closes proximity for least square method (LSM) and can be utilized as an approximation of $f(x)$ (especially when N is much bigger than n). Coefficients $a_0^*,...,a_n^*$ are a solution to the following linear algebraic system (which has a symmetric matrix and for its solution can be utilized square root method):

$$\left|\begin{array}{l} Na_0 + \left(\sum_{i=1}^{N} x_i\right)a_1 + \left(\sum_{i=1}^{N} x_i^2\right)a_2 + ... + \left(\sum_{i=1}^{N} x_i^n\right)a_n = \sum_{i=1}^{N} y_i \\ \left(\sum_{i=1}^{N} x_i\right)a_0 + \left(\sum_{i=1}^{N} x_i^2\right)a_1 + \left(\sum_{i=1}^{N} x_i^3\right)a_2 + ... + \left(\sum_{i=1}^{N} x_i^{n+1}\right)a_n = \sum_{i=1}^{N} x_i y_i \\ .... \\ \left(\sum_{i=1}^{N} x_i^n\right)a_0 + \left(\sum_{i=1}^{N} x_i^{n+1}\right)a_1 + \left(\sum_{i=1}^{N} x_i^{n+2}\right)a_2 + ... + \left(\sum_{i=1}^{N} x_i^{2n}\right)a_n = \sum_{i=1}^{N} x_i^n y_i \end{array}\right.$$

Analogically with least square method for approximation of the functions given in a table the following concept is introduced: “solution using least square method" for predetermined systems of linear algebraic equations (the number of equations *m* is larger than the number of unknowns *n*):

If the predetermined system is of the following type: $Ax = b$:

$$\begin{vmatrix} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n = b_n \end{vmatrix} \quad \text{for} \quad m > n.$$

A solution found using LSM is n – the point $(x_1^*,\ldots,x_n^*)$, which minimizes the expression:

$$\Phi(x_1,\ldots,x_n) = (a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n - b_1)^2 + (a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n - b_2)^2 + \ldots + (a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n - b_m)^2$$

The point which minimizes this function is a solution to the quadratic system which we get when we multiply the left side of the output system with A^T :$\boldsymbol{A^TAx = A^Tb}$, which is also called system symmetrization.

Example 1. Find P_1^* and P_2^* using LSM for the function $f(x)$ given in the table:

x_i	0	1	2	3	4
$y_i = f(x_i)$	1	2	1	0	4

Solution:

To find P_1^* we construct a table using the values of $x_i, y_i, x_i^2, y_i x_i$ and find the necessary totals:

i	x_i	y_i	x_i^2	$x_i y_i$
1	0	1	0	0
2	1	2	1	2
3	2	1	4	2
4	3	0	9	0
5	4	4	16	16
Σ	**10**	**8**	**30**	**20**

Then if $P_1^* = a_1^* x + a_0^*$ coefficients a_0^* and a_1^* are a solution to the system:

$$\begin{vmatrix} 5a_0 + 10a_1 = 8 \\ 10a_0 + 30a_1 = 20 \end{vmatrix},$$

the solutions to which are $a_0^* = \frac{4}{5}$ and $a_1^* = \frac{2}{5} \Rightarrow P_1^* = \frac{2}{5}x + \frac{4}{5}$.

To find the polynomial of degree two P_2^* we add three more columns to the table above: $x_i^3, x_i^4, y_i x_i^2$:

i	x_i	y_i	x_i^2	x_i^3	x_i^4	$x_i y_i$	$y_i x_i^2$
1	0	1	0	0	0	0	0
2	1	2	1	1	1	2	2
3	2	1	4	8	16	2	4
4	3	0	9	27	81	0	0
5	4	4	16	64	256	16	64
Σ	**10**	**8**	**30**	**100**	**354**	**20**	**70**

So the system is reduced to the form

$$\left|\begin{array}{l} 5a_0 + 10a_1 + 30a_2 = 8 \\ 10a_0 + 30a_1 + 100a_2 = 20 \\ 30a_0 + 100a_1 + 354a_2 = 70 \end{array}\right. .$$

The solutions of the system (with an accuracy of up to five digits) are: $a_0^* = 1{,}65714$; $a_1^* = -1{,}31429$; $a_2^* = 0{,}42857$ and $P_2^*(x) = 0{,}42857x^2 - 1{,}31429x + 1{,}65714$.

Example 2. Solve the predetermined system using LSM

$$\left|\begin{array}{l} x + y = 2 \\ x - y = 0 \\ 3x + y = 3 \end{array}\right. .$$

Solution:

The matrix $A = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 3 & 1 \end{pmatrix}$; $A^T = \begin{pmatrix} 1 & 1 & 3 \\ 1 & -1 & 1 \end{pmatrix}$ and the vector $b = \begin{pmatrix} 2 \\ 0 \\ 3 \end{pmatrix}$. Then

$$A^T A = \begin{pmatrix} 1 & 1 & 3 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 3 & 1 \end{pmatrix} = \begin{pmatrix} 11 & 3 \\ 3 & 3 \end{pmatrix}; \quad A^T b = \begin{pmatrix} 1 & 1 & 3 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \\ 3 \end{pmatrix} = \begin{pmatrix} 11 \\ 5 \end{pmatrix}.$$

And we get a symmetrized system: $\left|\begin{array}{l} 11x + 3y = 11 \\ 3x + 3y = 5 \end{array}\right.$.

After subtracting the second equation from the first one we have $8x = 6 \Rightarrow x = \frac{3}{4}$ and after the substitution $3y = 5 - \frac{9}{4} \Rightarrow y = \frac{11}{12}$, i.e. the solutions of the predetermined system are $x^* = \frac{3}{4}$ and $y^* = \frac{11}{12}$.

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