DATA APPROXIMATION

BY

POLYNOMIALS OF N-TH DEGREE

AND

SMALLEST SQUARES METHOD

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To develop general approximation formulas we will start from usual approximation of measurements by a polynomial of the second degree:

$$f(x)=ax^2+bx+c$$

In this particular example such function will be interpreted as function of three variables a, b and c, where x is constant:

$$F(a, b, c)=ax^2+bx+c$$

There's set of data from tests performed in lab, pointing dependency of physical value y from x. Data measurements are set of N pairs of x_i and relating to it values of y_i.

We lay the polynomial along measurements, so in moments x_i difference between polynomial and measured value is:

$$\Psi(a, b, c) = y_i-ax_i^2-bx_i-c$$

To get more precise approximation we square the difference:

$$\Psi(a, b, c) = (y_i-ax_i^2-bx_i-c)^2$$

and sum along all measurements from 1 to N:

$$\boldsymbol{F}(a, b, c)=\sum_{i=1}^{N}(y_i-ax^2-bx-c)^2$$

This function tells how far the polynomial goes off the measurement points, for each set of parameters a, b and c. The exercise is to find such set of a, b and c, that maintains smallest possible value of F(a, b, c), what means smallest possible deviation error after exchanging tests with polynomial.

Typical examples for optimalisation says, that the function can have a minimum at points where derivative is zero and changes the sign. Let's calculate partial derivative of our function F(a, b, c) to find parameters a, b and c, where error will be minimal.

First, let's square the formula at the sigma:

$$\Psi(a, b, c) = (y_i-ax_i^2-bx_i-c)^2=(y_i-ax_i^2-bx_i-c)(y_i-ax_i^2-bx_i-c)=$$
$$=y_i^2-ax_i^2y_i-bx_iy_i-cy_i-ax_i^2y_i+a^2x_i^4+abx_i^3+acx_i^2-bx_iy_i+abx_i^3+b^2x_i^2+bcx_i-cy_i+acx_i^2+bcx_i+c^2$$

Further, we calculate partial derivatives along a, b and c and match them to zero. Because derivative of sum is equal to sum of derivatives, we skip sigma now and proceed only on summed elements:

$$\frac{\partial \boldsymbol{F}(a,b,c)}{\partial a} = -x_i^2y_i -x_i^2y_i +2ax_i^4 +bx_i^3 +cx_i^2 +bx_i^3 +cx_i^2 =$$
$$= 2ax_i^4 +2bx_i^3 +2x_i^2(c-y_i) = 0$$

$$\frac{\partial \boldsymbol{F}(a,b,c)}{\partial b} = -x_iy_i +ax_i^3 -x_iy_i +ax_i^3 + 2bx_i^2 + 2cx_i =$$
$$= 2ax_i^3 +2bx_i^2 +2x_i(c-y_i) = 0$$

$$\frac{\partial \boldsymbol{F}(a,b,c)}{\partial c} = -y_i +ax_i^2 +bx_i -y_i +ax_i^2 +bx_i +2c =$$
$$= 2ax_i^2 +2bx_i -2y_i +2c = 0$$

From now on, x^n represents sum of measurements x_i from i=1, …, N - where each reading is shifted to the power of n before the summing. The same do y's. By arranging partial derivative formulas in set of equations, we get:

$$2ax^4 + 2bx^3 + 2x^2(c-y) = 0$$
$$2ax^3 + 2bx^2 + 2x(c-y) = 0$$
$$2ax^2 + 2bx - 2y + 2c = 0$$

$$2ax^4 + 2bx^3 + 2x^2(c-y) = 0$$
$$2ax^3 + 2bx^2 + 2x(c-y) = 0$$
$$2ax^2 + 2bx + 2(c-y) = 0$$

$$ax^4 + bx^3 + x^2c = x^2y$$
$$ax^3 + bx^2 + xc = xy$$
$$ax^2 + bx + c = y$$

This set can be represented in form of matrix equation:

$$\begin{bmatrix} x^4 & x^3 & x^2 \\ x^3 & x^2 & x \\ x^2 & x & N \end{bmatrix} \times \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} x^2 y \\ xy \\ y \end{bmatrix}$$

Vector of solutions is given after inverting matrix of powers:

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} x^4 & x^3 & x^2 \\ x^3 & x^2 & x \\ x^2 & x & N \end{bmatrix}^{-1} \times \begin{bmatrix} x^2 y \\ xy \\ y \end{bmatrix}$$

Quite similar one, for linear approximation looks like this:

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} x^2 & x \\ x & N \end{bmatrix}^{-1} \times \begin{bmatrix} xy \\ y \end{bmatrix}$$

Comparing with bigger form of matrix, one can develop general clue for approximation with polynomial of degree n:

$$\begin{bmatrix} a_n \\ a_{n-1} \\ \vdots \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} x^{2n} & x^{2n-1} & \cdots & x^n \\ x^{2n-1} & x^{2n-2} & \cdots & x^{n-1} \\ \vdots & \vdots & .\cdot\dot{} & \vdots \\ x^{n+1} & x^n & \cdots & x \\ x^n & x^{n-1} & \cdots & N \end{bmatrix}^{-1} \times \begin{bmatrix} x^n y \\ x^{n-1} y \\ \vdots \\ xy \\ y \end{bmatrix}$$

It may seem not clear how c in last equation transformed into N. c simply means cx^0, which is c times 1. Since we skipped sigma we have to recall that, we still count empty powers of x^0. And this simply is because:

$$\sum_{i=1}^{N} x_i^{\,0} = \sum_{i=1}^{N} 1 = N$$

Here goes the elaboration of symbols:

$a_n, a_{n-1}, \cdots, a_1, a_0$ - vector of polynomial coefficients solving the approximation; that's what we search for; generally measurement points are approximated with polynomial:

$$a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 = 0$$

$x^{2n}, x^{2n-1}, \cdots, x^n, \cdots, x^1$ - sums of measurement points – the arguments in domain; for approximation by a polynomial of n-th degree there are sums of 2n power of each measurement required

$x^n \equiv \sum_{i=1}^{N} x_i^n$ - each element of main matrix is sum of measurement moments altered to n-th power.

N - is the number of measurement points

$x^n y, x^{n-1} y, \cdots, xy, y$ - sums of particular powers of each measurement point multiplied by relevant measurement itself; simply multiplication of i.e. moment in time to n-th power, multiplied by a readout at that time, and all measurements are afterwards summed

$x^n y \equiv \sum_{i=1}^{N} x_i^n y_i$ - each of elements of last vector means sum of particular measurement moments, powered to n and multiplied by measured value. Sum is done along N measurement points.

$\boldsymbol{A}^{-1} = \frac{1}{det(\boldsymbol{A})} \cdot (\boldsymbol{A}^{\boldsymbol{D}})^{\boldsymbol{T}}$ - finding polynomial factors aims on calculating inversion of main matrix of equation. To reach this solution, one has to perform five steps:

1. Separate all minors of the matrix by crossing row and column for each element of it in succession
2. Calculate determinant of each minor and multiply by a checkers pattern - $(-1)^{i+j}$ to create matrix of algebraic complements; i is the number of row crossed-out and j is the number of crossed-out column; transposition of this matrix is not necessary, as it is symmetrical along the diagonal
3. Calculate determinant of the matrix by unwrapping it along one of rows or columns; multiply elements of one row or column by it's algebraic complements
4. Divide algebraically each of algebraic complements by the determinant within the matrix
5. Multiply the result by the last vector with measurement values ($x^n y, x^{n-1} y, \cdots, xy, y$)

What remains is solution in form of the vector, containing all following coefficients of polynomial that approximate measurements the best possible way.

If above method of calculating solutions seemed to tedious, there's another one. Determinants' method. First one has to calculate main determinant of a matrix, then by replacing each column by $x^n y, x^{n-1} y, \cdots, xy, y$, it is possible to find values of full set of parameters aligning the polynomial best way. In example for second degree polynomial:

$$\boldsymbol{W} = det \begin{vmatrix} x^4 & x^3 & x^2 \\ x^3 & x^2 & x \\ x^2 & x & N \end{vmatrix} \quad \boldsymbol{W}_{\boldsymbol{a}} = det \begin{vmatrix} x^2 y & x^3 & x^2 \\ xy & x^2 & x \\ y & x & N \end{vmatrix} \quad \boldsymbol{W}_{\boldsymbol{b}} = det \begin{vmatrix} x^4 & x^2 y & x^2 \\ x^3 & xy & x \\ x^2 & y & N \end{vmatrix} \quad \boldsymbol{W}_{\boldsymbol{c}} = det \begin{vmatrix} x^4 & x^3 & x^2 y \\ x^3 & x^2 & xy \\ x^2 & x & y \end{vmatrix}$$

The solutions are: $a=W_a/W$, $b=W_b/W$, $c=W_c/W$

In general:

$$W = det\begin{vmatrix} x^{2n} & x^{2n-1} & \cdots & x^n \\ x^{2n-1} & x^{2n-2} & \cdots & x^{n-1} \\ \vdots & \vdots & \iddots & \vdots \\ x^{n+1} & x^n & \cdots & x \\ x^n & x^{n-1} & \cdots & N \end{vmatrix} \quad W_{a_n} = det\begin{vmatrix} x^n y & x^{2n-1} & \cdots & x^n \\ x^{n-1} y & x^{2n-2} & \cdots & x^{n-1} \\ \vdots & \vdots & \iddots & \vdots \\ xy & x^n & \cdots & x \\ y & x^{n-1} & \cdots & N \end{vmatrix}$$

$$W_{a_{n-1}} = det\begin{vmatrix} x^{2n} & x^n y & \cdots & x^n \\ x^{2n-1} & x^{n-1} y & \cdots & x^{n-1} \\ \vdots & \vdots & \iddots & \vdots \\ x^{n+1} & xy & \cdots & x \\ x^n & y & \cdots & N \end{vmatrix} \quad W_{a_0} = det\begin{vmatrix} x^{2n} & x^{2n-1} & \cdots & x^n y \\ x^{2n-1} & x^{2n-2} & \cdots & x^{n-1} y \\ \vdots & \vdots & \iddots & \vdots \\ x^{n+1} & x^n & \cdots & xy \\ x^n & x^{n-1} & \cdots & y \end{vmatrix}$$

The same way here: $a_n=W_{an}/W$, $a_{n-1}=W_{an-1}/W$, … , $a_0=W_{a0}/W$

EXAMPLE:

We will approximate 5 measurements with polynomial of fourth degree.

This is measurement chart:

x	-0.4	-0.2	0	0.4	0.8
y	-0.17	-0.8	-1	-0.17	2.61

The approximating polynomial is: $ax^4+bx^3+cx^2+dx+e=0$

Let's add necessary powers to the list x2-x8 are second to eight powers of each measurement. Powers of measurements vector are also added.

n=5	1	2	3	4	5	Σ
x	-0.4	-0.2	0	0.4	0.8	0.6
y	-0.17	-0.8	-1	-0.17	2.61	0.46
x2	0.1600000000	0.0400000000	0.0000000000	0.1600000000	0.6400000000	1.0000000000
x3	-0.0640000000	-0.0080000000	0.0000000000	0.0640000000	0.5120000000	0.5040000000
x4	0.0256000000	0.0016000000	0.0000000000	0.0256000000	0.4096000000	0.4624000000
x5	-0.0102400000	-0.0003200000	0.0000000000	0.0102400000	0.3276800000	0.3273600000
x6	0.0040960000	0.0000640000	0.0000000000	0.0040960000	0.2621440000	0.2704000000
x7	-0.0016384000	-0.0000128000	0.0000000000	0.0016384000	0.2097152000	0.2097024000
x8	0.0006553600	0.0000025600	0.0000000000	0.0006553600	0.1677721600	0.1690854400
x4y	-0.0044646400	-0.0012774400	0.0000000000	-0.0044646400	1.0688921600	1.0586854400
x3y	0.0111616000	0.0063872000	0.0000000000	-0.0111616000	1.3361152000	1.3425024000
x2y	-0.0279040000	-0.0319360000	0.0000000000	-0.0279040000	1.6701440000	1.5824000000
xy	0.0697600000	0.1596800000	0.0000000000	-0.0697600000	2.0876800000	2.2473600000

Here's the matrix with written values from sigma column in measurement charts:

$$\begin{vmatrix} 0.1690854 & 0.2097024 & 0.2704000 & 0.3273600 & 0.4624000 \\ 0.2097024 & 0.2704000 & 0.3273600 & 0.4624000 & 0.5040000 \\ 0.2704000 & 0.3273600 & 0.4624000 & 0.5040000 & 1.0000000 \\ 0.3273600 & 0.4624000 & 0.5040000 & 1.0000000 & 0.6000000 \\ 0.4624000 & 0.5040000 & 1.0000000 & 0.6000000 & 5.0000000 \end{vmatrix}$$

And here is the matrix inverted:

$$\begin{vmatrix} 3607.856 & -2506.51 & -821.398 & 368.49 & 39.063 \\ -2506.51 & 1837.023 & 514.974 & -274.392 & -23.438 \\ -821.398 & 514.974 & 229.08 & -77.188 & -12.5 \\ 368.49 & -274.392 & -77.188 & 43.903 & 3.75 \\ 39.063 & -23.438 & -12.5 & 3.75 & 1 \end{vmatrix}$$

Now it is enough to multiply this inverted matrix by a vector $x^n y, x^{n-1} y, \cdots, xy, y$, and here's the result:

a	1.00
b	0.00
c	4.99
d	0.00
e	-1.00

Approximated polynomial is: $f(x)=x^4+4.99x^2-1$

By inserting measurements points into found function, we receive former values. This is prove for correctness of calculations:

$f(-0.4)=-0.4^4+4.99(-0.4)^2-1=0.0256+0.8-1=-0.17$

$f(0)=0+0-1=-1$