# Curve Fitting by the Method of Least Squares

Source: Applied Numerical Methods for the Micro Computer, Terry E. Shoup, Prentice Hall, Inc. New Jersey, 1984

given $n+1$ datapoints $(x_0, y_0) \cdots (x_n, y_n)$
over range $x_0 \le x \le x_n$
approximated by function $g(x)$

$$\text{Error}_i = g(x_i) - y_i$$

Sum of squares of errors are added, so that errors do not cancel each others by sign:

$$E = \sum_{i=\emptyset}^{n} [g(x_i) - y_i]^2$$

if $g(x) = c_1 g_1(x) + c_2 g_2(x) \cdots c_K g_K(x)$

$$\therefore \quad E = \sum_{i=\emptyset}^{n} [c_1 g_1(x_i) + c_2 g_2(x_i) \cdots c_K g_K(x_i)]^2$$

thus $\dfrac{\partial E}{\partial c_1} = \dfrac{\partial E}{\partial c_2} = \cdots = \dfrac{\partial E}{\partial c_K} = \emptyset$ for minimum $E$

if $g(x)$ are orthogonal polynomials such that

$$g_j(x_i)\, g_K(x_i) = \emptyset \qquad j \ne K$$

then $$c_j = \frac{\sum_{i=\emptyset}^{n} g_j(x_i) y_i}{\sum_{i=\emptyset}^{n} g_j^2(x_i)}$$

Can solve simultaneous equation using Cholesky's method (see next page)

Cholesky's method for simultaneous linear equations

1) The augmented matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \end{bmatrix}$$

can be presented in the form

$$U = \begin{bmatrix} 1 & U_{12} & U_{13} & U_{14} & U_{15} \\ 0 & 1 & U_{23} & U_{24} & U_{25} \\ 0 & 0 & 1 & U_{34} & U_{35} \\ 0 & 0 & 0 & 1 & U_{45} \end{bmatrix}$$

where

$$L = \begin{bmatrix} L_{11} & 0 & 0 & 0 \\ L_{21} & L_{22} & 0 & 0 \\ L_{31} & L_{32} & L_{33} & 0 \\ L_{41} & L_{42} & L_{43} & L_{44} \end{bmatrix}$$

and $[L][U] = [A]$

$$U_{1j} = a_{1j} / L_{11} \quad \text{for } j = 2, 3 \cdots n+1$$

**Parameters**

n = number of data points
KK = number of coefficients

**Arrays** X(n+1), Y(n+1), A(KK+1, KK+2), C(KK+1)

X(i), Y(i) for i = 1 to n — data points

**Find coefficients**

1) Load the "A" array

```
For L=1 to KK
   For M=1 to KK
      S1 = Ø
      S2 = Ø
      For I = 1 to N
         S1 = S1 + X(I)^(L-1) * X(I)^(M-1)
         S2 = S2 + X(I)^(L-1) * Y(I)
      Next N
      A(L,M) = S1
      A(L, KK +1) = S2
   Next M
Next L
```

2) Solve the equation using the Cholesky Method

```
NROW = KK
NCOL = KK+1
For K = 1 to NROW
   PIVOT = A(K,K) : IL = K
   FOR L = K+1 TO NROW
      IF ABS(A(L,K)) ≥ ABS(PIVOT) THEN [PIVOT = A(L,K) : IL=L]
   NEXT L
   IF IL <> K THEN BEGIN
      FOR LL = 1 TO NCOL
         TEMP = A(K,LL) : A(K,LL) = A(IL,LL) : A(IL,LL) = TEMP
      NEXT LL   END
NEXT K
```

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3) Calculate

```
FOR J = 2 TO NCOL
    A (1,J) = A (I,J) / A (1,1)
NEXT J
FOR L = 2 TO NROW
    FOR I = L TO NROW
        SUM = Ø
        FOR K = 1 TO L-1
            SUM = SUM + A (I,K) * A (K,L)
        NEXT K
        A (I,L) = A (I,L) - SUM
    NEXT I
    FOR J = L+1 TO NCOL
        SUM = Ø
        FOR K = 1 TO L-1
            SUM = SUM + A (L,K) * A (K,J)
        NEXT K
        A (L,J) = (A (L,J) - SUM) / A (L,L)
    NEXT J
NEXT L
```

4) Get Coefficients

```
C (NROW) = A (NROW, NCOL)
FOR M = 1 to NROW-1
    I = NROW - M
    SUM = Ø
    FOR J = I+1 TO NROW
        SUM = SUM + A (I,J) * C (J)
    NEXT J
    C (I) = A (I,NCOL) - SUM
NEXT M
```

The answer is in the form

$$Y = C(1) + C(2)*X + C(3)*X^2 + C(4)*X^3$$
$$\ldots \quad C(KK)*X\text{^}(KK-1)$$

in code;

```
Write('The answer is a polynomial of order ');
Write(KK-1)
Write(' of the following coefficients:')

For I := 1 to KK do Begin
    Write('C(');
    Write(I);
    Write('):');
    Writeln(C[I]);
    end;
```