CMPSC/Math 451, Numerical Computation

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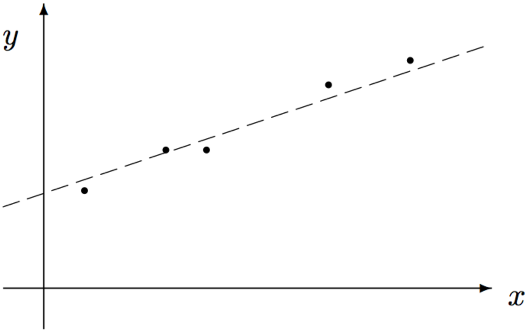
Given data set

x	x_0	x_1	x_2	$\cdots$	x_m
y	y_0	y_1	y_2	$\cdots$	y_M

Want to fit in a function $y = f(x)$
such that the error $e_k = f(x_k) - y_k$ is minimized.

Linear regression and basic derivation

We want to fit in $y(x) = ax + b$.



Problem:
Find a, b, such that when we use $y = ax + b$, the "error" becomes smallest possible.

How to measure error?

1. $\max_k |y(x_k) - y_k|$ — l_∞ norm
2. $\sum_{k=0}^{m} |y(x_k) - y_k|$ — l_1 norm
3. $\sum_{k=0}^{m} [y(x_k) - y_k]^2$ — l_2 norm, used in Least Square Method. (LSM)

A minimization problem:

Find a and b such that the error function $\psi(a, b)$ defined as

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

is minimized.

How to find a and b?

At the minimum of a function, we have

$$\frac{\partial \psi}{\partial a} = \frac{\partial \psi}{\partial b} = 0$$

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

$$\frac{\partial \psi}{\partial a} = 0 \quad : \quad \sum_{k=0}^{m} 2(a x_k + b - y_k) x_k = 0, \qquad (I)$$

$$\frac{\partial \psi}{\partial b} = 0 \quad : \quad \sum_{k=0}^{m} 2(a x_k + b - y_k) = 0, \qquad (II)$$

Solve $(I), (II)$ for (a,b). Rewrite it as a system

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

These are called the normal equations.

Example 1. Data set for S (liquid surface tension) and T (temperature)

T_k	0	10	20	30	40	80	90	95
S_k	68.0	67.1	66.4	65.6	64.6	61.8	61.0	60.0

From physics we know that they have a linear relation $S = aT + b$. Use MLS to find the best fitting a, b.

Answer. We have $m = 7$, and the sums:

$$\sum_{k=0}^{7} T_k^2 = 26525, \quad \sum_{k=0}^{7} T_k = 365, \quad \sum_{k=0}^{7} T_k S_k = 22685, \quad \sum_{k=0}^{7} S_k = 514.5.$$

$$\text{The normal equations:} \quad \left\{ \begin{array}{rcl} 26525\,a + 365\,b & = & 22685 \\ 365\,a + 8\,b & = & 514.5 \end{array} \right.$$

$$\text{Solve it:} \quad a = -0.079930, \qquad b = 67.9593.$$

Linear LSM with 3 functions

Given data set (x_k, y_k) for $k = 0, 1, \cdots, m$. Find a function

$$y(x) = a \cdot f(x) + b \cdot g(x) + c \cdot h(x)$$

which best fit the data.
This means we need to find (a, b, c).
Here $f(x), g(x), h(x)$ are given functions, for example

$$f(x) = e^x, \qquad g(x) = \ln(x), \qquad h(x) = \cos x,$$

but not restricted to these.

Define the error function:

$$\psi(a,b,c) = \sum_{k=0}^{m} (y(x_k) - y_k)^2 = \sum_{k=0}^{m} \left(a \cdot f(x_k) + b \cdot g(x_k) + c \cdot h(x_k) - y_k\right)^2$$

At minimum, we have

$$\frac{\partial \psi}{\partial a} = 0 \quad : \qquad \sum_{k=0}^{m} 2\Big[a \cdot f(x_k) + b \cdot g(x_k) + c \cdot h(x_k) - y_k\Big] \cdot f(x_k) = 0$$

$$\frac{\partial \psi}{\partial b} = 0 \quad : \qquad \sum_{k=0}^{m} 2\Big[a \cdot f(x_k) + b \cdot g(x_k) + c \cdot h(x_k) - y_k\Big] \cdot g(x_k) = 0$$

$$\frac{\partial \psi}{\partial c} = 0 \quad : \qquad \sum_{k=0}^{m} 2\Big[a \cdot f(x_k) + b \cdot g(x_k) + c \cdot h(x_k) - y_k\Big] \cdot h(x_k) = 0$$

The normal equations are

$$\begin{aligned}
\left(\sum_{k=0}^{m} f(x_k)^2\right) a + \left(\sum_{k=0}^{m} f(x_k)g(x_k)\right) b + \left(\sum_{k=0}^{m} f(x_k)h(x_k)\right) c &= \sum_{k=0}^{m} f(x_k)y_k \\
\left(\sum_{k=0}^{m} f(x_k)g(x_k)\right) a + \left(\sum_{k=0}^{m} g(x_k)^2\right) b + \left(\sum_{k=0}^{m} h(x_k)g(x_k)\right) c &= \sum_{k=0}^{m} g(x_k)y_k \\
\left(\sum_{k=0}^{m} f(x_k)h(x_k)\right) a + \left(\sum_{k=0}^{m} g(x_k)h(x_k)\right) b + \left(\sum_{k=0}^{m} h(x_k)^2\right) c &= \sum_{k=0}^{m} h(x_k)y_k
\end{aligned}$$

We note that the system of normal equations is always symmetric. We only need to compute half of the entries.

General linear LSM

Given data set (x_k, y_k), $k = 0, 1, \cdots, m$.
Let $g_0, g_1, g_2, \cdots g_n$ be $n+1$ given functions, linearly independent.
We search for a function in the form

$$y(x) = \sum_{i=0}^{n} c_i g_i(x)$$

that best fit the data.
Here g_i's are called *basis functions*.

Define error function

$$\psi(c_0, c_1, \cdots, c_n) = \sum_{k=0}^{m} \left[y(x_k) - y_k \right]^2 = \sum_{k=0}^{m} \left[\left(\sum_{i=0}^{n} c_i g_i(x_k) \right) - y_k \right]^2$$

At minimum, we have

$$\frac{\partial \psi}{\partial c_j} = 0, \qquad j = 0, 1, \cdots, n.$$

This gives:

$$\sum_{k=0}^{m} 2 \left[\left(\sum_{i=0}^{n} c_i g_i(x_k) \right) - y_k \right] g_j(x_k) = 0$$

Re-arranging the ordering of summation signs:

$$\sum_{i=0}^{n} \left(\sum_{k=0}^{m} g_i(x_k) g_j(x_k) \right) c_i = \sum_{k=0}^{m} g_j(x_k) y_k, \qquad j = 0, 1, \cdot, n.$$

$$\sum_{i=0}^{n}\left(\sum_{k=0}^{m} g_i(x_k)g_j(x_k)\right)c_i = \sum_{k=0}^{m} g_j(x_k)y_k, \qquad j = 0, 1, \cdot, n.$$

This gives the system of normal equations:

$$A\vec{c} = \vec{b}$$

where $\vec{c} = (c_0, c_1, \cdots, c_n)^t$ and

$$A = \{a_{ij}\}, \qquad a_{ij} = \sum_{k=0}^{m} g_i(x_k)g_j(x_k)$$

$$\vec{b} = \{b_j\}, \qquad b_j = \sum_{k=0}^{m} g_j(x_k)y_k.$$

We note that this A is symmetric, $a_{ij} = a_{ji}$.

Non-linear LSM: quasi-linear

Consider fitting the data set (x_k, y_k) with the function $y(x) = a \cdot b^x$.
This means, we need to find (a, b) such that this $y(x)$ best fit the data.

$$\text{variable change:} \qquad \ln y = \ln a + x \cdot \ln b\,.$$

Let

$$S = \ln y, \qquad \bar{a} = \ln a, \qquad \bar{b} = \ln b, \qquad \rightarrow \quad S(x) = \bar{a} + \bar{b}x.$$

Generate data (x_k, S_k) where $S_k = \ln y_k$ for all k.
Use linear LSM and find $(\bar{a}, \bar{b})$ such that $S(x)$ best fits (x_k, S_k).
Then, transform back to the original variable

$$a = \exp\{\bar{a}\}, \qquad b = \exp\{\bar{b}\}.$$

Non-linear LSM

For the data (x_k, y_k), fit in the function $y(x) = ax \cdot \sin(bx)$.
No variable change that can change this problem into a linear one.
The function arises in the solution of 2nd order ODE with resonance.
Define error

$$\psi(a,b) = \sum_{k=0}^{m} \Big[y(x_k) - y_k \Big]^2 = \sum_{k=0}^{m} \Big[ax_k \cdot \sin(bx_k) - y_k \Big]^2.$$

At minimum:

$$\frac{\partial \psi}{\partial a} = 0: \qquad \sum_{k=0}^{m} 2 \Big[ax_k \cdot \sin(bx_k) - y_k \Big] \cdot [x_k \cdot \sin(bx_k)] = 0$$

$$\frac{\partial \psi}{\partial b} = 0: \qquad \sum_{k=0}^{m} 2 \Big[ax_k \cdot \sin(bx_k) - y_k \Big] \cdot [ax_k \cdot \cos(bx_k)x_k] = 0$$

$\to 2 \times 2$ system of non-linear equations to solve for (a, b)!
May use Newton's method to find a root. May not have unique solution.

Least square for continuous functions

Problem. Given: function $f(x)$ on $x \in [a, b]$,
and a set of basis functions g_i $(i = 1, 2, \cdots, n)$ on $x \in [a, b]$.

Find a function: $$g(x) = \sum_{i=1}^{n} a_i g_i(x)$$

to minimize the error: $$E(f, g) = \|f - g\|_2^2 = \int_a^b (f(x) - g(x))^2 \, dx$$

This means: $$E(a_1, a_2, \cdots, a_n) = \int_a^b \left(f(x) - \sum_{i=1}^{n} a_i g_i(x) \right)^2 d$$

At the minimum, we must have

$$\frac{\partial E}{\partial a_i} = 0, \qquad i = 1, 2, \cdots, n$$

$$E(a_1, a_2, \cdots, a_n) = \int_a^b \left(f(x) - \sum_{i=1}^{n} a_i g_i(x) \right)^2 \, dx.$$

$$\begin{aligned} \frac{\partial E}{\partial a_i} &= -2 \int_a^b g_i(x) \left(f(x) - \sum_{j=1}^{n} a_j g_j(x) \right) \, dx = 0 \\ & \int_a^b g_i(x) f(x) \, dx - \int_a^b g_i(x) \sum_{j=1}^{n} a_j g_j(x) \, dx = 0 \end{aligned}$$

we have

$$\sum_{j=1}^{n} a_j \int_a^b g_i(x) g_j(x) \, dx = \int_a^b g_i(x) f(x) \, dx, \qquad i = 1, 2, \cdots n$$

$$\sum_{j=1}^{n} a_j \int_a^b g_i(x) g_j(x)\, dx = \int_a^b g_i(x) f(x)\, dx, \qquad i = 1, 2, \cdots n$$

Writing this into matrix-vector form:

$$C\vec{a} = \vec{b}$$

where

$$C = \{c_{ij}\}, \quad c_{ij} = \int_a^b g_i(x) g_j(x)\, dx, \qquad b_i = \int_a^b g_i(x) f(x)\, dx.$$

Note that the matrix C is symmetric, since $c_{ij} = c_{ji}$.
If the basis functions $\{g_i\}$ are linearly independent, then the matrix C is non-singular, and the system $C\vec{a} = \vec{b}$ has a unique solution.

Orthogonal basis.

If the basis function $g_i(x)$ are orthogonal to each other, i.e., if $i \neq j$, then

$$\int_a^b g_i(x)g_j(x)\,dx = 0, \qquad \rightarrow \qquad c_{ij} = 0$$

then the C matrix is diagonal, and the system is trivial to solve.

$$c_{ii} = \int_a^b (g_i(x))^2\,dx, \qquad a_i = \frac{b_i}{a_{ii}} = \frac{\int_a^b g_i(x)f(x)\,dx}{\int_a^b (g_i(x))^2\,dx}.$$

Examples of families of orthogonal functions

Legendre polynomials

For interval $[-1,1]$, they are

$$
\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= (3x^2 - 1)/2, \\
P_3(x) &= (5x^3 - 3x)/2, \\
P_4(x) &= (35x^4 - 30x^2 + 3)/8, \\
&\cdots
\end{aligned}
$$

They are solutions to Legendre equation.

Example 1. Verify that $P_o = 1, P_1 = x, P_2 = (3x^2 - 1)/2$ are orthogonal to each other.
Answer. Note: P_0, P_2 are even functions, and P_1 is odd.
Then, $P_0(x)P_1(x)$ and $P_1(x)P_2(x)$ are odd.

$$\int_{-1}^{1} P_0(x)P_1(x)\,dx = 0, \qquad \int_{-1}^{1} P_1(x)P_2(x)\,dx = 0.$$

We only need to check

$$\int_{-1}^{1} P_0(x)P_2(x)\,dx = \frac{1}{2}\int_{-1}^{1}(3x^2 - 1)\,dx = \frac{1}{2}(x^3 - x)\Big|_{-1}^{1} = 0,$$

proving that P_0, P_1, P_2 are orthogonal to each other.

Example 2. Find a function $g(x) = a_0 P_0(x) + a_1 P_1(x) + a_2 P_2(x)$ on $-1 \leq x \leq 1$, that "best" approximates the function

$$f(x) = \begin{cases} -1, & -1 \leq x \leq 0 \\ 1, & 0 < x \leq 1 \end{cases} .$$

Answer. With orthogonal basis, the coefficients a_i are simply computed as

$$a_i = \frac{\int_{-1}^{1} f(x) P_i(x)\, dx}{\int_{-1}^{1} P_i^2(x)\, dx}.$$

Note that $f(x)$ is odd, therefore $f(x)P_0(x)$ and $f(x)P_2(x)$are odd, and $a_0 = 0,\ a_2 = 0$. We only need to compute a_1:

$$a_1 = \frac{\int_{-1}^{1} f(x) P_1(x)\, dx}{\int_{-1}^{1} P_1^2(x)\, dx} = \frac{2\int_0^1 x\, dx}{\int_{-1}^{1} x^2\, dx} = \frac{2(0.5)}{2/3} = \frac{3}{2}.$$

Therefore, the "best" approximation is $\quad g(x) = \frac{3}{2} P_1(x) = \frac{3}{2} x.$

From Differential Equation Course, we learned that the set of trig functions, defined on the interval $x \in [-\pi, \pi]$,

$$1, \sin nx, \cos nx, \quad n = 1, 2, \cdots$$

are orthogonal to each other. This means,

$$\begin{aligned}
\int_{-\pi}^{\pi} 1 \cdot \sin nx \, dx &= 0, && \text{for every} \quad n \\
\int_{-\pi}^{\pi} 1 \cdot \cos nx \, dx &= 0, && \text{for every} \quad n \\
\int_{-\pi}^{\pi} \sin nx \cdot \sin mx \, dx &= 0 && \text{for every} \quad m \neq n \\
\int_{-\pi}^{\pi} \cos nx \cdot \cos mx \, dx &= 0 && \text{for every} \quad m \neq n \\
\int_{-\pi}^{\pi} \sin nx \cdot \cos mx \, dx &= 0 && \text{for every} \quad m, n
\end{aligned}$$

Example 4. Given M. Approximate a function $f(x)$ defined on $[-\pi,\pi]$ by

$$g(x) = c_0 + \sum_{n=1}^{M} \Big[a_n \sin nx + b_n \cos nx \Big],$$

in the "best" possible way.

Answer. Using the orthogonal property, the coefficients are computed as

$$a_n = \frac{\int_{-\pi}^{\pi} f(x) \sin nx \, dx}{\int_{-\pi}^{\pi} \sin^2 nx \, dx}, \qquad b_n = \frac{\int_{-\pi}^{\pi} f(x) \cos nx \, dx}{\int_{-\pi}^{\pi} \cos^2 nx \, dx}$$

$$c_0 = \frac{1}{2} \int_{-\pi}^{\pi} f(x) \, dx.$$

As $M \to \infty$, we obtain the Fourier series for $f(x)$!