ORTHOGONALITY & CURVE FITTING - Prof. Richard B. Goldstein

Fitting Continuous Functions by Polynomials: f(x) on [a, b]

Minimize $\displaystyle\int_a^b \left[f(x) - \left\{a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m\right\}\right]^2 dx$

Example #1: $f(x) = e^x$ on [-1, 1] can be represented by $a_0 + a_1 x + a_2 x^2$

Solve:

$$\begin{aligned}
a_0\int_{-1}^{1} 1\,dx &+ a_1\int_{-1}^{1} x\,dx + a_2\int_{-1}^{1} x^2\,dx = \int_{-1}^{1} e^x\,dx = e - e^{-1}\\
a_0\int_{-1}^{1} x\,dx &+ a_1\int_{-1}^{1} x^2\,dx + a_2\int_{-1}^{1} x^3\,dx = \int_{-1}^{1} xe^x\,dx = 2e^{-1}\\
a_0\int_{-1}^{1} x^2\,dx &+ a_1\int_{-1}^{1} x^3\,dx + a_2\int_{-1}^{1} x^4\,dx = \int_{-1}^{1} x^2e^x\,dx = e - 5e^{-1}
\end{aligned}$$

Solution: $e^x \approx 0.996294 + 1.103638x + 0.536721x^2$

Why use orthogonal polynomials?

[1] Higher degree polynomial fits have nearly singular matrices. For example, if a continuous curve is fit on the interval [0, 1] using powers of x: $1, x, x^2, x^3, \ldots, x^m$, the resulting matrix of the coefficients is the **Hilbert Matrix**:

$$A_m = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{m} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{m+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{1}{m} & \frac{1}{m+1} & \frac{1}{m+2} & \cdots & \frac{1}{2m-1} \end{bmatrix}$$

$\lvert A_2\rvert$	= 1/12	$= 8.33 \times 10^{-2}$
$\lvert A_3\rvert$	= 1/2,160	$= 4.63 \times 10^{-4}$
$\lvert A_4\rvert$	= 1/6,048,000	$= 1.65 \times 10^{-7}$
$\lvert A_5\rvert$		$= 3.75 \times 10^{-12}$
…		
$\lvert A_{10}\rvert$		$= 2.16 \times 10^{-53}$

[2] The coefficient matrix becomes simplified to a diagonal matrix making the coefficients easy to find once the orthogonal polynomials have been chosen.

An orthogonal set of polynomials on [-1, 1]

Legendre Polynomials

$P_0(x) = 1,\ P_1(x) = x,\ P_2(x) = \frac{3}{2}x^2 - \frac{1}{2},\ P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x, \ldots$

where $\left\langle P_j, P_k \right\rangle = \displaystyle\int_{-1}^{1} P_j(x)P_k(x)\,dx = \begin{cases} \frac{2}{2k+1} & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases}$

and $(k+1)P_{k+1}(x) = (2k+1)xP_k(x) - kP_{k-1}(x)$ is the recursion generating equation

$f(x) \approx a_0P_0(x) + a_1P_1(x) + \cdots + a_mP_m(x)$ where $a_k = \dfrac{\left\langle P_k, f(x)\right\rangle}{\left\langle P_k, P_k\right\rangle} = \frac{2k+1}{2}\displaystyle\int_{-1}^{1} P_k(x)f(x)\,dx$

Example #2: (repeating example #1 with orthogonal polynomials)

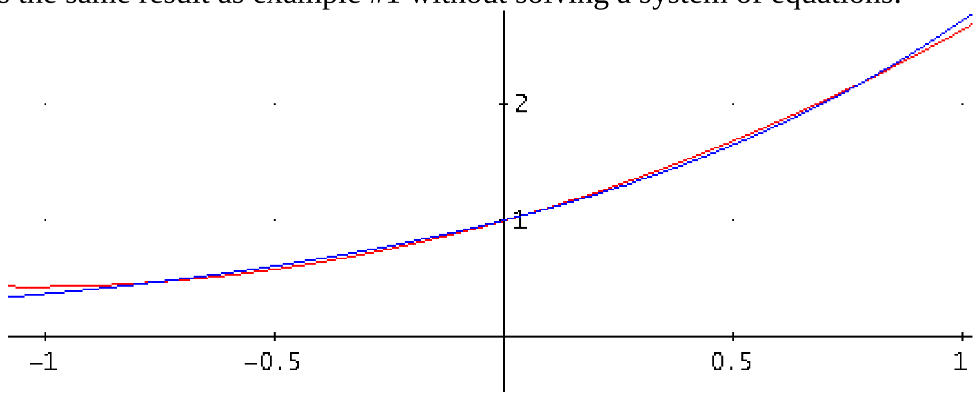
Then, $\frac{1}{2}\langle f(x), P_0(x)\rangle = \frac{1}{2}\left(e - e^{-1}\right) \approx 1.175201$,

$\frac{3}{2}\langle f(x), P_1(x)\rangle = \frac{3}{2}\left(2e^{-1}\right) \approx 1.103638$,

and $\frac{5}{2}\langle f(x), P_2(x)\rangle = \frac{5}{2}\left(e - 7e^{-1}\right) \approx 0.357814$

$$e^x \approx 1.175201 + 1.103638x + 0.357814\left(\tfrac{3}{2}x^2 - \tfrac{1}{2}\right) = 0.996294 + 1.103638x + 0.536721x^2$$

This is the same result as example #1 without solving a system of equations.



Note that the cubic term can be found by adding $a_3P_3(x)$ where $a_3 = \frac{7}{2}\int_{-1}^{1} P_3(x)f(x)\,dx$

Fitting Discrete Data by Orthogonal Polynomials:

Finding a set of orthogonal polynomials on the set of x's: $x_1, x_2, \ldots, x_n$

Let $\Phi_k(x) = k^{th}$ degree polynomial where $\sum_i \Phi_k(x_i)\Phi_\ell(x_i) = \langle \Phi_k, \Phi_\ell\rangle = 0$ if $k \neq \ell$

MODEL: $a_0\Phi_0(x_i) + a_1\Phi_1(x_i) + \ldots + a_m\Phi_m(x_i)$

$$\Phi_0(x) = 1$$
$$\Phi_1(x) = x - B_1 = x - \bar{x}$$
$$\Phi_k(x) = (x - B_k)\Phi_{k-1}(x) - C_k\Phi_{k-2}(x)$$

where $B_k = \dfrac{\sum_i x_i\Phi_{k-1}^2(x_i)}{\sum_i \Phi_{k-1}^2(x_i)}$ $\quad C_k = \dfrac{\sum_i x_i\Phi_{k-2}(x_i)\Phi_{k-1}(x_i)}{\sum_i \Phi_{k-2}^2(x_i)}$

$$a_k = \frac{\langle y, \Phi_k\rangle}{\langle \Phi_k, \Phi_k\rangle} = \frac{\sum_i y_i\Phi_k(x_i)}{\sum_i \Phi_k^2(x_i)}$$

Example #3: Find $\Phi_0(x)$, $\Phi_1(x)$, $\Phi_2(x)$ for x_i : -7, 2, 3, 5, 6, 9

Start with $\Phi_0(x) = 1$.

Next, $B_1 = \frac{\sum x_i \Phi_0^2(x_i)}{\sum \Phi_0^2(x_i)} = \frac{(-7)(1)^2 + (2)(1)^2 + (3)(1)^2 + (5)(1)^2 + (7)(1)^2 + (9)(1)^2}{(1)^2 + (1)^2 + (1)^2 + (1)^2 + (1)^2 + (1)^2} = \frac{18}{6} = 3$

Therefore, $\Phi_1(x) = x - 3$ Now, compute B_2 and C_2

$$B_2 = \frac{\sum x_i \Phi_1^2(x_i)}{\sum \Phi_1^2(x_i)} = \frac{(-7)(-10)^2 + (2)(-1)^2 + (3)(0)^2 + (5)(2)^2 + (7)(3)^2 + (9)(6)^2}{(-10)^2 + (-1)^2 + (0)^2 + (2)^2 + (3)^2 + (6)^2} = \frac{-300}{150} = -2$$

$$C_2 = \frac{\sum x_i \Phi_1(x_i)\Phi_0(x_i)}{\sum \Phi_0^2(x_i)} = \frac{(-7)(-10)1 + (2)(-1)1 + (3)(0)1 + (5)(2)1 + (7)(3)1 + (9)(6)1}{(1)^2 + (1)^2 + (1)^2 + (1)^2 + (1)^2 + (1)^2} = \frac{150}{6} = 25$$

Then, $\Phi_2(x) = (x-3)(x-(-2)) - 25 = (x-3)(x+2) - 25 = x^2 - x - 31$

Note that the vectors: [1, 1, 1, 1, 1, 1], [-10, -1, 0, 2, 3, 6] and [25, -29, -25, -11, -1, 41] are mutually orthogonal. These are the vectors of $\Phi_0(x_i)$, $\Phi_1(x_i)$, $\Phi_2(x_i)$

FURTHER DISCUSSION

[1] How do you choose the best m, since as m increases, the sum of squares always decreases? *Answer*: use Gauss' Criterion: minimize $\frac{\text{Sum Sqs}}{n-(m+1)}$

[2] Are there other criteria for a "best fit?" Yes – minimum absolute deviation. This is usually accomplished by starting with Tchebychev Polynomials.

ADVANCED PROBLEM: Fit $f(x) = 2^x$ on [0, 1] using

[A] 6 points x_i : 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0
[B] the continuous interval [0, 1]

[A] DISCRETE CASE

x_i	y_i	$\Phi_0(x_i)$	$\Phi_1(x_i)$	$\Phi_2(x_i)$	$\Phi_3(x_i)$
0.0	1.000 000 00	1	-0.5	+0.133 333 33	-0.0240
0.2	1.148 698 36	1	-0.3	-0.026 666 67	+0.0336
0.4	1.319 507 91	1	-0.1	-0.106 666 67	+0.0192
0.6	1.515 716 57	1	+0.1	-0.106 666 67	-0.1092
0.8	1.741 101 13	1	+0.3	-0.026 666 67	-0.0336
1.0	2.000 000 00	1	+0.5	+0.133 333 33	+0.0240

Start with $\boxed{\Phi_0(x) = 1}$

$$B_1 = \frac{\sum x_i (\Phi_0)^2}{\sum (\Phi_0)^2} = \frac{\sum x_i (1)^2}{\sum (1)^2} = \frac{3}{6} = 0.5 \rightarrow \boxed{\Phi_1(x) = x - 0.5}$$

$$B_2 = \frac{\sum x_i(\Phi_1)^2}{\sum(\Phi_1)^2} = \frac{0(-0.5)^2 + 0.2(-0.3)^2 + 0.4(-0.1)^2 + 0.6(0.1)^2 + 0.8(0.3)^2 + 1(0.5)^2}{(-0.5)^2 + (-0.3)^2 + (-0.1)^2 + (0.1)^2 + (0.3)^2 + (0.5)^2}$$

$$\left.\begin{array}{l} = \frac{0.35}{0.7} = 0.5 \\ C_2 = \frac{\sum x_i \Phi_0 \Phi_1}{\sum \Phi_0^2} = \frac{0.7}{6} \end{array}\right\} \rightarrow \quad \Phi_2(x) = (x - 0.5)(x - 0.5) - 0.1166\overline{6}$$

$$\boxed{\Phi_2(x) = x^2 - x + 0.133\overline{3}}$$

$$\left.\begin{array}{l} B_3 = \frac{\sum x_i \Phi_2^2}{\sum \Phi_2^2} = \frac{0.02986\overline{6}}{0.05973\overline{3}} = 0.5 \\ C_3 = \frac{\sum x_i \Phi_1 \Phi_2}{\sum \Phi_1^2} = \frac{0.05973\overline{3}}{0.7} = 0.0853\overline{3} \end{array}\right\} \rightarrow \quad \Phi_3(x) = (x - 0.5)(x^2 - x + 0.133\overline{3}) - 0.0853\overline{3}(x - 0.5)$$

$$\boxed{\Phi_3(x) = x^3 - 1.5x^2 + 0.548x - 0.024}$$

The coefficient matrix (A) is found using

$$\begin{bmatrix} n & 0 & 0 & 0 & \\ 0 & \sum \Phi_1^2 & 0 & 0 & \\ 0 & 0 & \sum \Phi_2^2 & 0 & \\ 0 & 0 & 0 & \sum \Phi_3^2 & \\ & & & & \ddots \end{bmatrix} = \begin{bmatrix} 6 & 0 & 0 & 0 & \\ 0 & 0.7 & 0 & 0 & \\ 0 & 0 & 0.05973\overline{3} & 0 & \\ 0 & 0 & 0 & 0.0041472 & \\ & & & & \ddots \end{bmatrix}$$

$$\sum \Phi_0(x_i) y_i = 8.725\,023\,96$$
$$\sum \Phi_1(x_i) y_i = 0.697\,341\,70$$
$$\sum \Phi_2(x_i) y_i = 0.020\,514\,74$$
$$\sum \Phi_3(x_i) y_i = 0.000\,328\,06$$

Coefficients:

$$a_0 = \frac{8.72502396}{6} = 1.45417066$$

$$a_1 = \frac{0.69734170}{0.7} = 0.99620243$$

$$a_2 = \frac{0.02051474}{0.05973333} = 0.34343873$$

$$a_3 = \frac{0.00032806}{0.0041472} = 0.07910397$$

Model: $1.45417066(1) + 0.96620243(x - 0.5) + 0.34343873(x^2 - x + 0.1333333)$
$+0.07910397(x^3 - 1.5x^2 + 0.548x - 0.024) + \ldots$

2 terms: $0.95606945 + 0.99620243x$

3 terms: $1.00186128 + 0.65276370x + 0.34343873x^2$

4 terms: $0.99996278 + 0.69611268x + 0.22478278x^2 + 0.07910397x^3$

note: $1 + (\ln 2)x + \frac{(\ln 2)^2}{2!}x^2 + \frac{(\ln 2)^3}{3!}x^3 + \ldots$ is the Taylor Series expansion about a = 0.

[B] CONTINUOUS CASE

Transform Legendre Polynomials from [-1, 1] to [a, b] by letting $x = \left(\frac{2}{b-a}\right)t - \left(\frac{b+a}{b-a}\right)$

In this example, since a = 0 and b = 1, then x = 2t -1. Now, $\langle P_k(t), P_k(t)\rangle = \frac{b-a}{2k+1}$. This leads to $P_0(t) = 1,\ P_1(t) = x = 2t-1,\ P_2(t) = \frac{3x^2-1}{2} = 6t^2 - 6t + 1,\ P_3(t) = 20t^3 - 30t^2 + 12t - 1$

Next, find $\langle P_k(t), 2^t\rangle = \int_0^1 P_k(t)2^t\,dt$. The results which were found using ***Derive*** are shown in the matrix on the right:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{5} & 0 \\ 0 & 0 & 0 & \frac{1}{7} \end{bmatrix}\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\ln 2} \\ \frac{3}{\ln 2} - \frac{2}{(\ln 2)^2} \\ \frac{1}{\ln 2} - \frac{18}{(\ln 2)^2} + \frac{12}{(\ln 2)^3} \\ \frac{3}{\ln 2} - \frac{12}{(\ln 2)^2} + \frac{180}{(\ln 2)^3} - \frac{120}{(\ln 2)^4} \end{bmatrix} = \begin{bmatrix} 1.44269504 \\ 0.16534716 \\ 0.011421868 \\ 0.00056405072 \end{bmatrix}$$

Solving, a_0 = 1.44269504, a_1 = 0.49604148, a_2 = 0.057109340, and a_3 = 0.0039483550

The resulting fit is for

2 terms:	1.44269504 + 0.49604148(2t – 1) = 0.94665356 + 0.99208296t
3 terms:	$1.00376290 + 0.64942692t + 0.34265604t^2$
4 terms:	$0.99981455 + 0.69680718t + 0.22420539t^2 + 0.07896710t^3$

Sum Squares for each case are as follows:

Case	**Discrete Case**	**Continuous Case**
2 terms	7.072×10^{-3}	6.543×10^{-4}
3 terms	2.599×10^{-5}	2.232×10^{-6}
4 terms	3.943×10^{-8}	4.248×10^{-9}