Continuous Least-Square Fit

We want to find the 'best' way of approximating $\sin x$ by a quadratic polynomial, in the interval $0 < x < \frac{\pi}{2}$ (let's work in radians now).

We do it again by minimizing the 'sum' (now the integral) of squares of the residuals:

$$S = \int_0^{\pi/2} \left(\sin x - a - b\,x - c\,x^2\right)^2 dx$$

or

$$S = \int_A^B \left(y(x) - a - b\,x - c\,x^2\right)^2 dx$$

in general.

This leads to the following **normal equations** for a, b and c

$$\left.\begin{array}{ccc} \int_A^B dx & \int_A^B x\,dx & \int_A^B x^2 dx \\ \int_A^B x\,dx & \int_A^B x^2 dx & \int_A^B x^3 dx \\ \int_A^B x^2 dx & \int_A^B x^3 dx & \int_A^B x^4 dx \end{array}\right\| \begin{array}{c} \int_A^B y(x)dx \\ \int_A^B x\,y(x)\,dx \\ \int_A^B x^2 y(x)\,dx \end{array}$$

Important simplification is achieved by first assuming: $A = -1$ and $B = 1$. This is not a real restriction - we can easily go from $y(x)$ to $Y(X) \equiv y\left(\frac{A+B}{2} + \frac{B-A}{2}X\right)$, and back, by the so called **shift**: $X \to \frac{2x-(A+B)}{B-A}$.

We can thus concentrate on solving

$$\left.\begin{array}{ccc} \int_{-1}^{1} dX & \int_{-1}^{1} X\,dX & \int_{-1}^{1} X^2 dX \\ \int_{-1}^{1} X\,dX & \int_{-1}^{1} X^2 dX & \int_{-1}^{1} X^3 dX \\ \int_{-1}^{1} X^2 dX & \int_{-1}^{1} X^3 dX & \int_{-1}^{1} X^4 dX \end{array}\right\| \begin{array}{c} \int_{-1}^{1} Y(X)dX \\ \int_{-1}^{1} X\ \cdot Y(X)\,dX \\ \int_{-1}^{1} X^2 \cdot Y(X)\,dX \end{array}$$

Secondly, instead of using $a + b\,X + c\,X^2$, we will fit

$$\hat{a}\,\phi_0(X) + \hat{b}\,\phi_1(X) + \hat{c}\,\phi_2(X)$$

where $\phi_0(X)$, $\phi_1(X)$ and $\phi_2(X)$ are zero, first and second degree polynomials, *orthogonal* in the following sense:

$$\int_{-1}^{1} \phi_i(X) \cdot \phi_j(X)\,dX = 0$$

whenever $i \neq j$.

This modifies our normal equations to

$$\begin{array}{ccc|c} \int_{-1}^{1} {\phi_0}^2 dX & \int_{-1}^{1} \phi_0\phi_1 \, dX & \int_{-1}^{1} \phi_0\phi_1 \, dX & \int_{-1}^{1} \phi_0 Y dX \\ \int_{-1}^{1} \phi_1\phi_0 \, dX & \int_{-1}^{1} {\phi_1}^2 dX & \int_{-1}^{1} \phi_1\phi_2 \, dX & \int_{-1}^{1} \phi_1 Y \, dX \\ \int_{-1}^{1} \phi_2\phi_0 \, dX & \int_{-1}^{1} \phi_2\phi_1 \, dX & \int_{-1}^{1} {\phi_2}^2 dX & \int_{-1}^{1} \phi_2 Y \, dX \end{array}$$

with all the off-diagonal elements equal to *zero*. The solution is thus quite trivial:

$$\begin{aligned} \hat{a} &= \frac{\int_{-1}^{1} \phi_0(X)Y(X)dX}{\alpha_0} \\ \hat{b} &= \frac{\int_{-1}^{1} \phi_1(X)Y(X)dX}{\alpha_1} \\ \hat{c} &= \frac{\int_{-1}^{1} \phi_2(X)Y(X)dX}{\alpha_2} \end{aligned}$$

where $\alpha_0 \equiv \int_{-1}^{1} \phi_0(X)^2 dX$, $\alpha_1 \equiv \int_{-1}^{1} \phi_1(X)^2 dX$, etc.

Furthermore, to fit a cubic polynomial instead of quadratic, we simply add

$$\hat{d} = \frac{\int_{-1}^{1} \phi_3(X)Y(X)dX}{\alpha_3}$$

Typical error:

$$\sqrt{\frac{S_{\text{min}}}{2}} = \sqrt{\frac{\int_{-1}^{1} Y(X)^2 dX - \alpha_0 \, \hat{a}^2 - \alpha_1 \, \hat{b}^2 - \alpha_2 \, \hat{c}^2}{2}}$$

Orthogonal (Legendgre) Polynomials:

We must yet construct ϕ_0, ϕ_1, ϕ_2, ...

We start with

$$\phi_0(X) = 1$$

(any constant would do); the corresponding α_0 is: $\int_{-1}^{1} 1^2\, dX = 2$.

Next, we try $\phi_1(X) = X + C$. Making it orthogonal to $\phi_0(X)$ requires

$$\int_{-1}^{1} 1 \cdot (X + C)\, dX = 2C = 0$$

which implies that $C = 0$. We thus have

$$\phi_1(X) = X$$

with $\alpha_1 = \int_{-1}^{1} X^2\, dX = \frac{2}{3}$.

At this point we may realize that polynomials containing only odd powers of X are *automatically* orthogonal to polynomials with only even powers. Utilizing that: $\phi_2(X) = X^2 + C$ (different C). It is automatically orthogonal to $\phi_1(X)$, we must also make it orthogonal to $\phi_0(X)$ by

$$\int_{-1}^{1} 1 \cdot (X^2 + C)\, dX = \frac{2}{3} + 2C = 0 \Rightarrow C = -\frac{1}{3}$$

This results in

$$\phi_2(X) = X^2 - \frac{1}{3}$$

with $\alpha_2 = \int_{-1}^{1} (X^2 - \frac{1}{3})^2\, dX = \frac{2}{5} - \frac{4}{9} + \frac{2}{9} = \frac{8}{45}$ (the $\int_{-1}^{1} X^{2n}\, dX = \frac{2}{2n+1}$ formula comes handy).

Similarly, $\phi_3(X) = X^3 + C\, X$. Making it orthogonal to $\phi_1(X)$:

$$\int_{-1}^{1} X \cdot (X^3 + C\, X)\, dX = \frac{2}{5} + \frac{2}{3}C = 0 \Rightarrow C = -\frac{3}{5}$$

Thus

$$\phi_3(X) = X^3 - \frac{3}{5}\, X$$

and $\alpha_3 = \int_{-1}^{1} (X^3 - \frac{3}{5}X)^2\, dX = \frac{2}{7} - \frac{6}{5} \cdot \frac{2}{5} + \frac{9}{25} \cdot \frac{2}{3} = \frac{8}{175}$.

To construct $\phi_4(X)$ we can use $X^4 + C_2 X^2 + C_0$, but it is more convenient (why?) to use $\phi_4(X) = X^4 + C_2 \phi_2(X) + C_0 \phi_0(X)$ instead. We have to make it orthogonal to $\phi_0(x)$:

$$\int_{-1}^{1} \phi_0(X) \cdot \left[X^4 + C_2\phi_2(X) + C_0\phi_0(X)\right] \, dX =$$

$$\frac{2}{5} + 2C_0 = 0 \Rightarrow C_0 = -\frac{1}{5}$$

and to $\phi_2(X)$:

$$\int_{-1}^{1} \phi_2(X) \cdot \left[X^4 + C_2\phi_2(X) + C_0\phi_0(X)\right] \, dX =$$

$$\frac{2}{7} - \frac{1}{3} \cdot \frac{2}{5} + \frac{8}{45}C_1 = 0 \Rightarrow C_1 = -\frac{6}{7}$$

implying that

$$\phi_4(X) = X^4 - \frac{6}{7}\left(X^2 - \frac{1}{3}\right) - \frac{1}{5} = X^4 - \frac{6}{7}X^2 + \frac{3}{35}$$

(the signs will always alternate), with $\alpha_4 = \int_{-1}^{1}(X^4 - \frac{6}{7}X^2 + \frac{3}{35})^2 \, dX = \frac{128}{11025}$.

It should be obvious, how to continue this process (called **Gram-Schmidt orthogonalization**). The resulting polynomials are called **Legendre**, and are quite useful in many other areas of Mathematics and Physics.

Example:

Fit $\sin x$ by a **cubic** polynomial, in the $(0, \frac{\pi}{2})$ interval.

Replacing x by $\frac{A+B}{2} + \frac{B-A}{2}X = \frac{\pi}{4}(1+X)$, this is the same as fitting $\sin[\frac{\pi}{4}(1+X)]$ over $(-1, 1)$.

Using the previous formulas:

$$\hat{a} = \frac{\int_{-1}^{1} \sin[\frac{\pi}{4}(1+X)] \, dX}{2} = \frac{2}{\pi}$$

$$\hat{b} = \frac{\int_{-1}^{1} X \sin[\frac{\pi}{4}(1+X)] \, dX}{\frac{2}{3}} = 6 \cdot \frac{4-\pi}{\pi^2}$$

$$\hat{c} = \frac{\int_{-1}^{1} (X^2 - \frac{1}{3}) \sin[\frac{\pi}{4}(1+X)] \, dX}{\frac{8}{45}} = -15 \cdot \frac{48 - 12\pi - \pi^2}{\pi^3}$$

$$\hat{d} = \frac{\int_{-1}^{1} (X^3 - \frac{3}{5}X) \sin[\frac{\pi}{4}(1+X)] \, dX}{\frac{8}{175}} = -35 \cdot \frac{960 - 240\pi - 24\pi^2 + \pi^3}{\pi^4}$$

The corresponding least-squares polynomial is thus

$$\frac{2}{\pi} + 6 \cdot \frac{4-\pi}{\pi^2}\, X - 15 \cdot \frac{48 - 12\pi - \pi^2}{\pi^3}(X^2 - \frac{1}{3})$$
$$-35 \cdot \frac{960 - 240\pi - 24\pi^2 + \pi^3}{\pi^4}(X^3 - \frac{3}{5}X)$$

having the typical error of

$$\sqrt{\frac{\int_{-1}^{1} \sin[\frac{\pi}{4}(1+X)]^2\, dX - 2\hat{a}^2 - \frac{2}{3}\hat{b}^2 - \frac{8}{45}\hat{c}^2 - \frac{8}{175}\hat{d}^2}{2}}$$

$$= 0.000833$$

The final answer must be expressed in terms of x (by: $X \to \frac{4}{\pi} \cdot x - 1$). Expanded, this yields:

$$-2.25846\,244 \times 10^{-3} + 1.02716\,9553x$$
$$-0.069943\,7654x^2 - 0.11386\,84594x^3$$