Course: Mathematical Modeling

Chapter: [2]

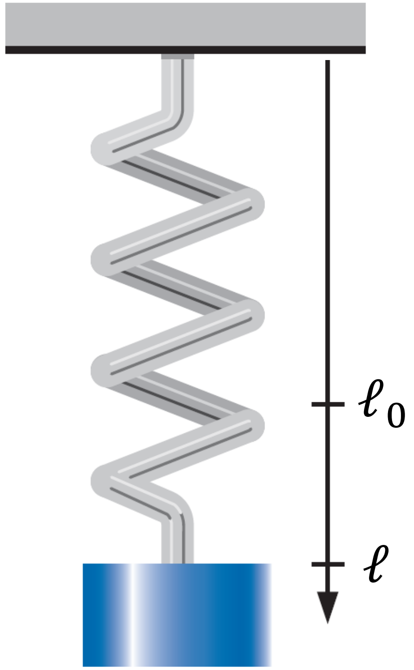
Model Fitting

Section: [*]

ITRODUCTION

DATA APPROXIMATION

Example **Hooke's law** states that when a force is applied to a spring constructed of uniform material, the length of the spring is a linear function of that force.



$$F(l) = k(\ell - \ell_0)$$

k is the spring constant

ℓ_0 is the length of the spring

ℓ is the length stretched by the force F

We want to determine the spring constant for a spring that has initial length 5.3 in.

Force (lb.)	Length (in.)
2	7.0
4	9.4
6	12.3

DATA APPROXIMATION

Example **Hooke's law** states that when a force is applied to a spring constructed of uniform material, the length of the spring is a linear function of that force.

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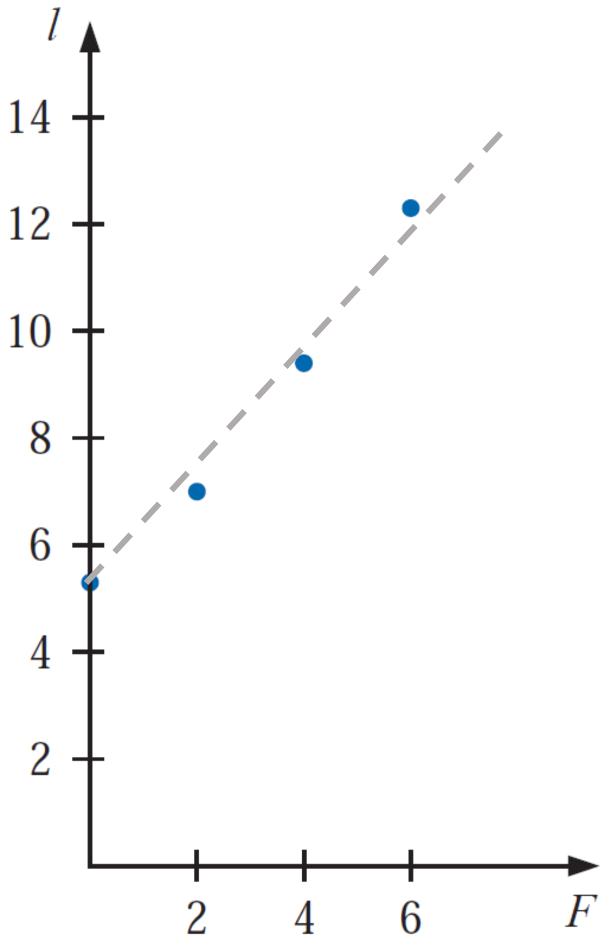


It is more reasonable to find the line that <u>best</u> approximates all the data points to determine the constant k.

APPROXIMATION THEORY

Two Types

[1] INTERPOLATION الاستيفاء

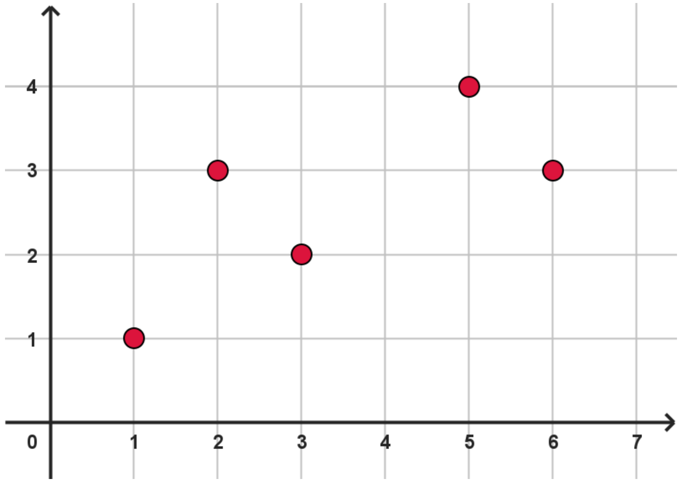
One problem arises when a function is given explicitly, but we wish to find a **simpler** type of function, such as a polynomial, to approximate values of the given function.

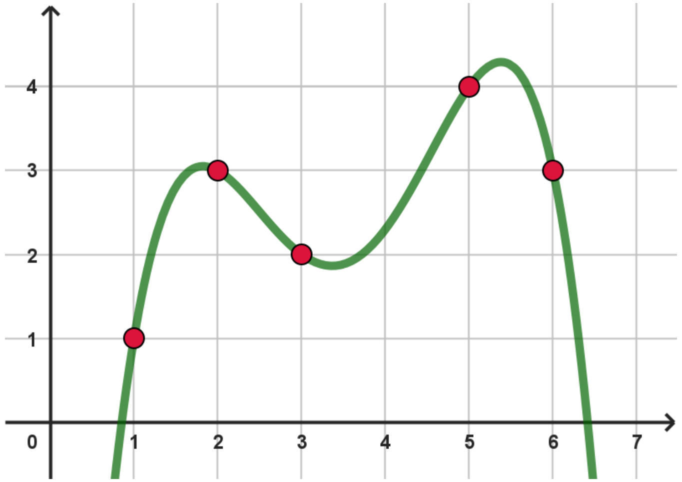
[2] FITTING CURVES الملاءمة

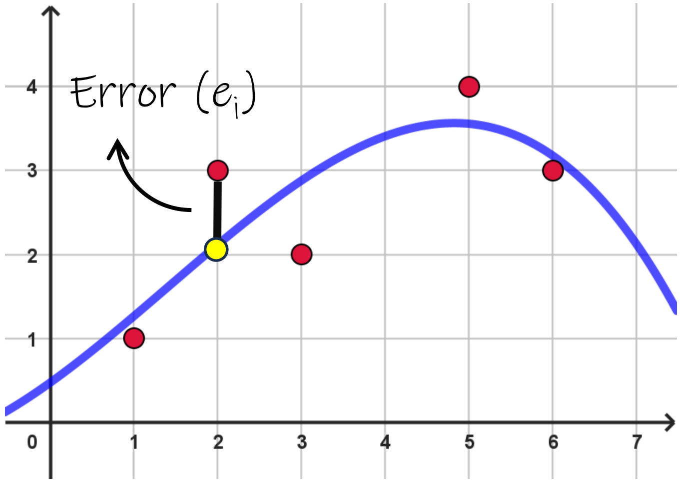
The other problem is concerned with fitting functions to given data and finding the **best** function in a certain class to represent the data.

MODEL FITTING vs INTERPOLATION

Idea **Interpolation** and **curve fitting** both generate new data points from known ones, but differ in *purpose*, *method*, and *application*.







(x_0, y_0)

(x_1, y_1)

$\vdots$

(x_n, y_n)

INTERPOLATION

1. Passing all points
2. Polynomial of degree at most n
3. Poor in approximating extrapolating data

CURVE FITTING

1. Not necessarily passing through the points (ERROR)
2. Any type of functions
3. Good in approximating other data

SOURCES OF ERROR IN THE MODELING PROCESS

[1] FORMULATION ERROR

Formulation errors arise from assuming some variables are unimportant or oversimplifying relationships between variables in different sub-models.

[2] MEASUREMENT ERROR

Measurement errors are obtained by a measuring instrument or process.

[3] ROUND-OFF ERROR

Round-off errors are caused by using a finite digit machine for computation.

$$\pi \approx 3.1415$$

[4] TRUNCATION ERROR

Truncation error arises when we cut off (truncate) an infinite process.

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} - \cdots$$

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Chapter: [2]

Model Fitting

Section: [2.1]

THE LEAST SQUARES METHOD

REVIEW OF 1ST ORDER PARTIAL DERIVATIVES

Definition Let $z = f(x, y)$ be a function of two variables. Then:

The Partial Derivative with respect to x:

$$\frac{\partial z}{\partial x} = f_x = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

The Partial Derivative with respect to y:

$$\frac{\partial z}{\partial y} = f_y = \lim_{\Delta y \to 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

REVIEW OF 1ST ORDER PARTIAL DERIVATIVES

Evaluation If $z = f(x, y)$ is a function of two variables. Then:

To find f_x Differentiate f with respect to x while treating y as a constant.

To find f_y Differentiate f with respect to y while treating x as a constant.

Example Find f_x and f_y for $f(x, y) = 4x^3 + 2x^2y + y^2$

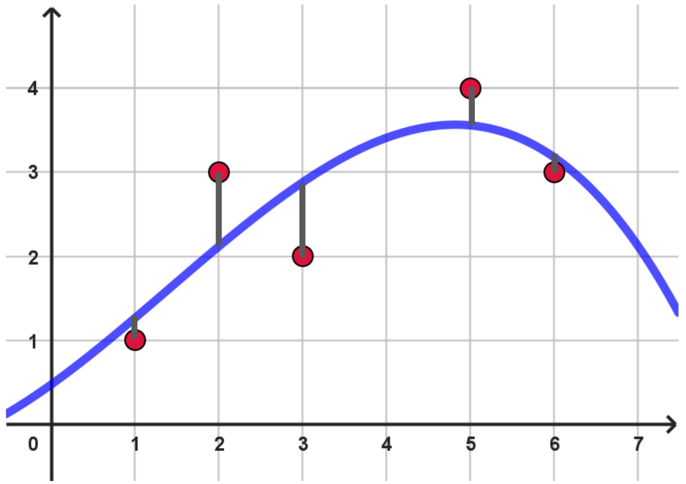
$$f_x(x, y) = \frac{\partial}{\partial x}(4x^3 + 2x^2y + y^2) = 12x^2 + 4xy$$

$$f_y(x, y) = \frac{\partial}{\partial y}(4x^3 + 2x^2y + y^2) = 2x^2 + 2y$$

DISCRETE LEAST SQUARES METHOD

The Idea In **curve fitting** we are given n points $(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$ and we want to determine a function $f(x)$ such that

$$y_1 \approx f(x_1) \longrightarrow e_1 = |y_1 - f(x_1)|$$
$$y_2 \approx f(x_2) \longrightarrow e_2 = |y_2 - f(x_2)|$$
$$\vdots$$
$$y_n \approx f(x_n) \longrightarrow e_n = |y_n - f(x_n)|$$



The function $f(x)$ should be fitted through the given points so that **<u>the sum of the squares</u>** of the **<u>distances</u>** of those points from $f(x)$ is **minimum**.

$$\min \sum_{i=1}^{n} (e_i)^2 = \min \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$$

THE PROCESS OF DISCRETE LEAST SQUARES METHOD

Linear Function

Suppose we want to fit the n points $(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$ by a linear function $f(x) = a + bx$.

$$q = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 = \sum_{i=1}^{n} (y_i - a - bx_i)^2$$

Find "**a**" and "**b**" such that "**q**" is **minimum**

Since q depends on a and b, then a *necessary* condition for q to be **minimum** is

$$\frac{\partial q}{\partial a} = 0 \longrightarrow -2\sum_{i=1}^{n} (y_i - a - bx_i) = 0$$

$$\frac{\partial q}{\partial b} = 0 \longrightarrow -2\sum_{i=1}^{n} (y_i - a - bx_i)(x_i) = 0$$

THE PROCESS OF DISCRETE LEAST SQUARES METHOD

Linear Function

$$-2\sum_{i=1}^{n}(y_i - a - bx_i) = 0 \rightarrow \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} a - b\sum_{i=1}^{n} x_i = 0$$

$$\rightarrow \boxed{an + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i} \quad \cdots (1)$$

$$-2\sum_{i=1}^{n}(y_i - a - bx_i)(x_i) = 0 \rightarrow \sum_{i=1}^{n} x_i y_i - a\sum_{i=1}^{n} x_i - b\sum_{i=1}^{n} x_i^2 = 0$$

$$\rightarrow \boxed{a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i} \quad \cdots (2)$$

THE PROCESS OF DISCRETE LEAST SQUARES METHOD

Linear Function

$$an + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

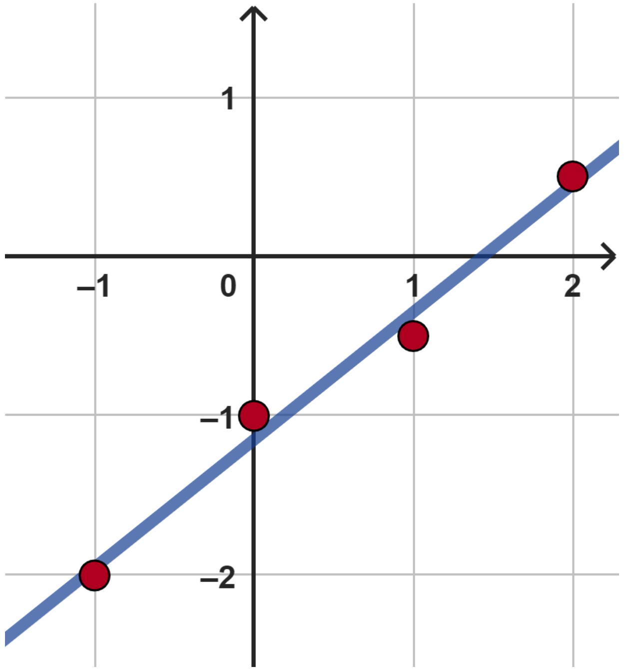
Example Find the linear function $f(x) = a + bx$ that best fits the following 4 points: $(-1,-2), (0,-1), \left(1,-\frac{1}{2}\right), \left(2,\frac{1}{2}\right)$

x_i	y_i	x_i^2	$x_i y_i$
-1	-2	1	2
0	-1	0	0
1	-0.5	1	-0.5
2	0.5	4	1
2	-3	6	2.5

$$\underbrace{\begin{aligned} 4a + 2b &= -3 \\ 2a + 6b &= 2.5 \end{aligned}}$$

$$\boxed{a = -1.15} \quad \boxed{b = 0.8}$$

$$\therefore f(x) = -1.15 + 0.8x$$



CURVE FITTING BY POLYNOMIALS OF DEGREE m

Process Given n points $(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$. Our method of curve fitting can be generalized to a polynomial of degree $m \leq n - 1$:

$$P_m(x) = b_0 + b_1 x + b_2 x^2 + \cdots + b_m x^m$$

Then $$q = \sum_{i=1}^{n} \left(y_i - P_m(x_i)\right)^2 = \sum_{i=1}^{n} (y_i - b_0 - b_1 x_i - \cdots - b_m x_i^m)^2$$

Since q depends on the parameters $b_0, b_1, \cdots, b_m$, then q is **minimum** if:

$$\frac{\partial q}{\partial b_0} = 0 \qquad \frac{\partial q}{\partial b_1} = 0 \qquad \cdots \qquad \frac{\partial q}{\partial b_m} = 0$$

CURVE FITTING BY POLYNOMIALS OF DEGREE m

Example Find the linear function $f(x) = a + bx + cx^2$ that best fits the following 5 points: $(-2,-1), (-1,2), (0,3), (1,2), (2,-1)$.

$$q = \sum_{i=1}^{n} \left(y_i - a - bx_i - cx_i^2\right)^2$$

$$\frac{\partial q}{\partial a} = 0 \quad \longrightarrow \quad -2\sum_{i=1}^{n} \left(y_i - a - bx_i - cx_i^2\right) = 0$$

$$\frac{\partial q}{\partial b} = 0 \quad \longrightarrow \quad -2\sum_{i=1}^{n} \left(y_i - a - bx_i - cx_i^2\right)(x_i) = 0$$

$$\frac{\partial q}{\partial c} = 0 \quad \longrightarrow \quad -2\sum_{i=1}^{n} \left(y_i - a - bx_i - cx_i^2\right)\left(x_i^2\right) = 0$$

CURVE FITTING BY POLYNOMIALS OF DEGREE m

Example Find the linear function $f(x) = a + bx + cx^2$ that best fits the following 5 points: $(-2,-1), (-1,2), (0,3), (1,2), (2,-1)$.

$$\sum_{i=1}^{n}(y_i - a - bx_i - cx_i^2) = 0 \longrightarrow an + b\sum x_i + c\sum x_i^2 = \sum y_i$$

$$\sum_{i=1}^{n}(y_i - a - bx_i - cx_i^2)(x_i) = 0 \longrightarrow a\sum x_i + b\sum x_i^2 + c\sum x_i^3 = \sum x_i y_i$$

$$\sum_{i=1}^{n}(y_i - a - bx_i - cx_i^2)(x_i^2) = 0 \longrightarrow a\sum x_i^2 + b\sum x_i^3 + c\sum x_i^4 = \sum x_i^2 y_i$$

CURVE FITTING BY POLYNOMIALS OF DEGREE m

Example Find the linear function $f(x) = a + bx + cx^2$ that best fits the following 5 points: $(-2,-1), (-1,2), (0,3), (1,2), (2,-1)$.

x_i	y_i	x_i^2	x_i^3	x_i^4	$x_i y_i$	$x_i^2 y_i$
-2	-1	4	-8	16	2	-4
-1	2	1	-1	1	-2	2
0	3	0	0	0	0	0
1	2	1	1	1	2	2
2	-1	4	8	16	-2	-4
0	5	10	0	34	0	-4

$$an + b\sum x_i + c\sum x_i^2 = \sum y_i$$

$$a\sum x_i + b\sum x_i^2 + c\sum x_i^3 = \sum x_i y_i$$

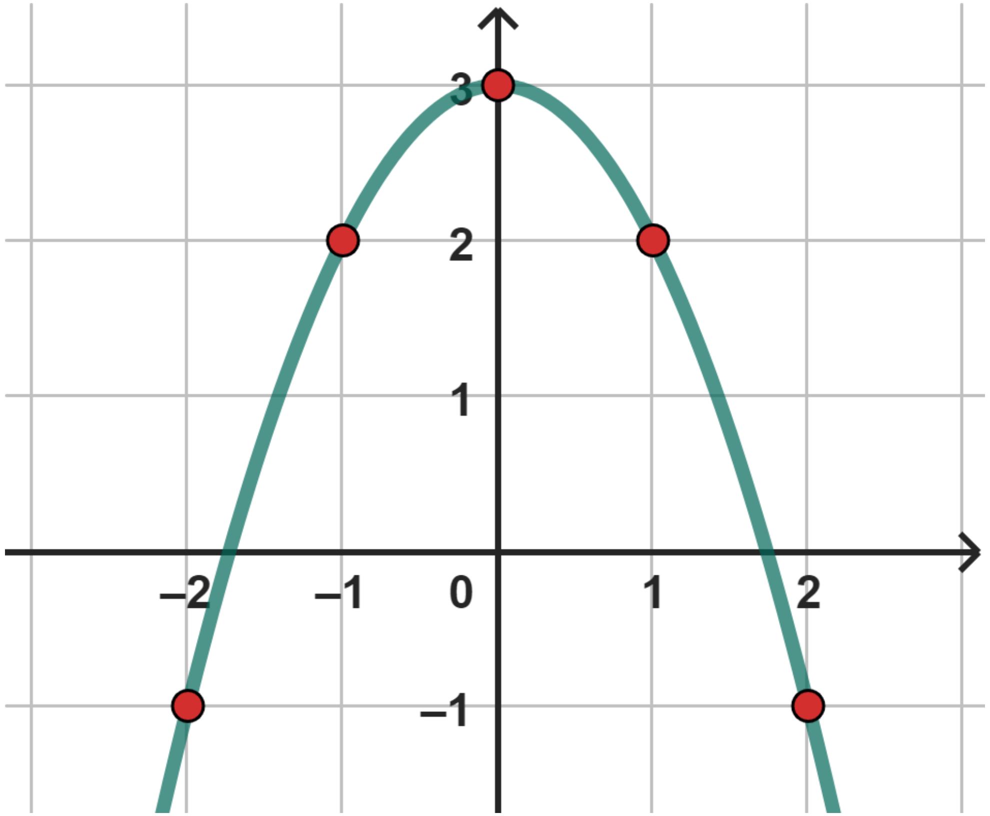
$$a\sum x_i^2 + b\sum x_i^3 + c\sum x_i^4 = \sum x_i^2 y_i$$

CURVE FITTING BY POLYNOMIALS OF DEGREE m

Example Find the linear function $f(x) = a + bx + cx^2$ that best fits the following 5 points: $(-2,-1), (-1,2), (0,3), (1,2), (2,-1)$.

$$\left.\begin{aligned} 5a + 10c &= 5 \\ b &= 0 \\ 10a + 34c &= -4 \end{aligned}\right\} \quad \begin{aligned} a &= 3 \\ b &= 0 \\ c &= -1 \end{aligned}$$

$$\therefore f(x) = 3 - x^2$$



CURVE FITTING BY GENERAL FUNCTIONS

Example Find the best function that fits the following data points and is of the form $f(x) = a\sin(\pi x) + b\cos(\pi x)$:

x	-1	$\frac{-1}{2}$	0	$\frac{1}{2}$	1
y	-1	0	1	2	1

$n = 5$

$$q = \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 = \sum_{i=1}^{n} (y_i - a\sin(\pi x_i) - b\cos(\pi x_i))^2$$

$$\boxed{\frac{\partial q}{\partial a} = 0} \longrightarrow \quad -2\sum_{i=1}^{5} (y_i - a\sin(\pi x_i) - b\cos(\pi x_i))(\sin(\pi x_i)) = 0$$

$$\boxed{\frac{\partial q}{\partial b} = 0} \longrightarrow \quad -2\sum_{i=1}^{5} (y_i - a\sin(\pi x_i) - b\cos(\pi x_i))(\cos(\pi x_i)) = 0$$

CURVE FITTING BY GENERAL FUNCTIONS

Example Find the best function that fits the following data points and is of the form $f(x) = a\sin(\pi x) + b\cos(\pi x)$:

x	y
-1	-1
$\frac{-1}{2}$	0
0	1
$\frac{1}{2}$	2
1	1

$$\sum_{i=1}^{5}\left(y_i\sin(\pi x_i) - a\sin^2(\pi x_i) - b\sin(\pi x_i)\cos(\pi x_i)\right) = 0$$

$$a\sum_{i=1}^{5}\sin^2(\pi x_i) + b\sum_{i=1}^{5}\sin(\pi x_i)\cos(\pi x_i) = \sum_{i=1}^{5} y_i\sin(\pi x_i)$$

$$\sum_{i=1}^{5}\left(y_i\cos(\pi x_i) - a\sin(\pi x_i)\cos(\pi x_i) - b\cos^2(\pi x_i)\right) = 0$$

$$a\sum_{i=1}^{5}\sin(\pi x)\cos(\pi x_i) + b\sum_{i=1}^{5}\cos^2(\pi x_i) = \sum_{i=1}^{5} y_i\cos(\pi x_i)$$

CURVE FITTING BY GENERAL FUNCTIONS

Example Find the best function that fits the following data points and is of the form $f(x) = a\sin(\pi x) + b\cos(\pi x)$:

x	y	$\sin(\pi x)$	$\cos(\pi x)$	$\sin^2(\pi x)$	$\cos^2(\pi x)$	$\sin(\pi x)\cos(\pi x)$	$y\sin(\pi x)$	$y\cos(\pi x)$
-1	-1	0	-1	0	1	0	0	1
$\frac{-1}{2}$	0	-1	0	1	0	0	0	0
0	1	0	1	0	1	0	0	1
$\frac{1}{2}$	2	1	0	1	0	0	2	0
1	1	0	-1	0	1	0	0	-1
				2	3	0	2	1

CURVE FITTING BY GENERAL FUNCTIONS

Example Find the best function that fits the following data points and is of the form $f(x) = a\sin(\pi x) + b\cos(\pi x)$:

$\sin^2(\pi x)$	$\cos^2(\pi x)$	$\sin(\pi x)\cos(\pi x)$	$y\sin(\pi x)$	$y\cos(\pi x)$
2	3	0	2	1

$$a\sum_{i=1}^{5}\sin^2(\pi x) + b\sum_{i=1}^{5}\sin(\pi x)\cos(\pi x) = \sum_{i=1}^{5} y_i\sin(\pi x_i) \longrightarrow a = 1$$

$$a\sum_{i=1}^{5}\sin(\pi x)\cos(\pi x) + b\sum_{i=1}^{5}\cos^2(\pi x) = \sum_{i=1}^{5} y_i\cos(\pi x_i) \longrightarrow b = \frac{1}{3}$$