

Research Methodology Tools:

1. Numerical Methods

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NA is an 'art' because the choice of appropriate procedure which 'best' suits to a given problem yields 'good' solutions.

Type Approach in Mathematics

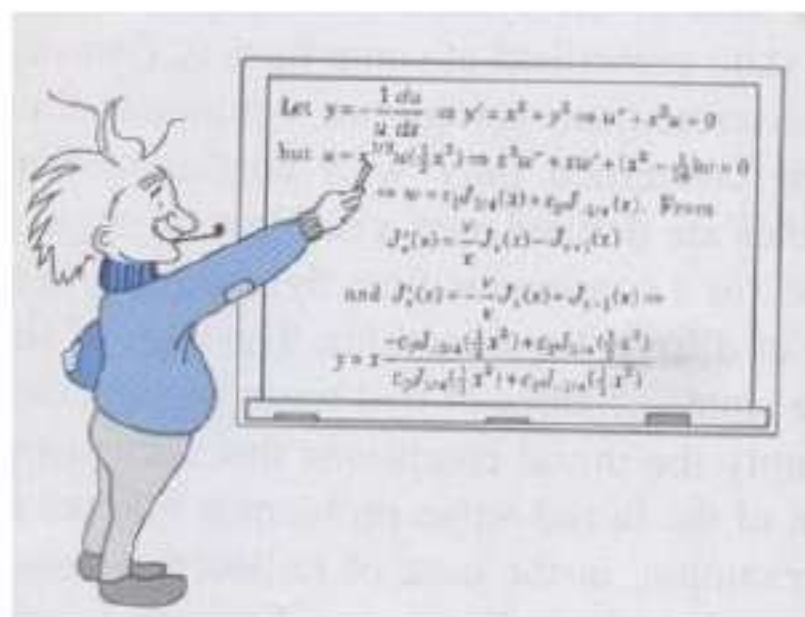


Figure: (a) Analytical approach

Type Approach in Mathematics



Figure: (a) Qualitative approach

Type Approach in Mathematics

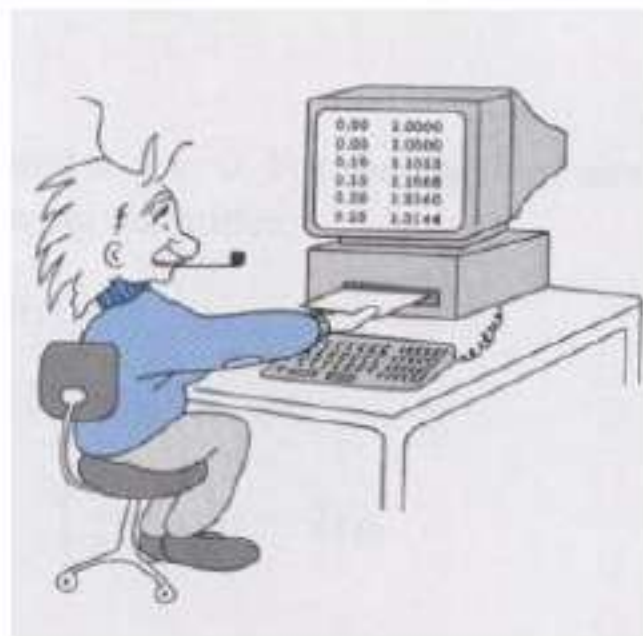


Figure: (a) Numerical approach

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(a) For a single variable function

$$f(x + \delta x) = f(x) + \delta x f'(x) + \frac{\delta x^2}{2} f''(x) + \frac{\delta x^3}{3!} f'''(x) + \dots \quad (1)$$

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(b) In two variables function

$$\begin{aligned} f(x + \delta x, y + \delta y) = & f(x, y) + \delta x f_x + \delta y f_y + \frac{\delta x^2}{2} \frac{\partial^2 f}{\partial x^2} \\ & + \frac{\delta y^2}{2} \frac{\partial^2 f}{\partial y^2} + \delta x \delta y \frac{\partial^2 f}{\partial x \partial y} + \dots \end{aligned} \quad (2)$$

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Similar expansions may be constructed for functions with more independent variables.

1. Bisection Method

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Consider the equation

$$f(x) = 0 \tag{3}$$

in $[x_a, x_b]$ and assume $f_a = f(x_a)$ and $f_b = f(x_b)$ such that $f_a f_b \leq 0$.

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in $[x_a, x_b]$ and assume $f_a = f(x_a)$ and $f_b = f(x_b)$ such that $f_a f_b \leq 0$. Clearly, if $f_a f_b = 0$ then one or both of x_a and x_b must be a root of $f(x) = 0$.

Root finding in one dimension

The procedure of Bisection method described in Figure below.

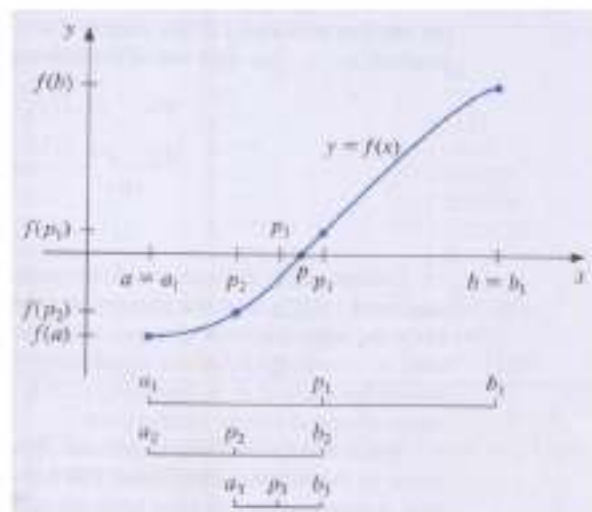


Figure: Bisection method

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By replacing the interval (x_a, x_b) with either (x_a, x_c) or (x_c, x_b) (whichever brackets the root), the error in our estimate of the solution to $f(x) = 0$ is, on average, halved. We repeat this interval halving until either the exact root has been found or the interval is smaller than some specified tolerance, $\epsilon > 0$.

1.1. Convergence

This method based on the intermediate theorem.

Since the interval (x_a, x_b) is halved for each iteration, then

$$\epsilon_n \sim \frac{e_n}{2}. \quad (4)$$

More generally, if x_n is the estimate for the root x^* at the n th iteration, then the error in this estimate is

$$\epsilon_n = x_n - x^*. \quad (5)$$

In many cases we may express the error at the $(n + 1)$ th time step in terms of the error at the n th time step as

$$|\epsilon_{n+1}| \sim C|\epsilon_n|^P. \quad (6)$$

The exponent P in equation (6) gives the order of the convergence. The larger the value of P , the faster the scheme converges on the solution, at least provided $n + 1 < n$. For first order schemes (i.e. $p = 1$), $|C| < 1$ for convergence.

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When using computer to generate approximations, it is a good practice to set an upper bound on the number of iterations. The best stopping criterion is

$$\frac{|x_n - x_{n-1}|}{|x_n|} < \epsilon \quad (7)$$

because it comes closest to testing relative error.

2.2 Bisection Algorithm

To find a solution $f(x)$ given continuous function f on the interval $[a, b]$, where $f(a)$ and $f(b)$ have opposite signs.

INPUT: Endpoints a, b ; tolerance TOL; maximum number of iterations N_0 .

2.2 Bisection Algorithm

To find a solution $f(x)$ given continuous function f on the interval $[a, b]$, where $f(a)$ and $f(b)$ have opposite signs.

INPUT: Endpoints a, b ; tolerance TOL; maximum number of iterations N_0 .

OUTPUT: approximate solution x^* or message of failure.

Step 1 Set $i = 1$. $FA = f(a)$

Step 2 While $i \leq N_0$ do Step 2.1 - 2.4.

Step 2.1 Set $x = a + \frac{b-a}{2}$; $FX = f(x)$
(Compute x_i)

Step 2.2 If $FX = 0$ or $\frac{b-a}{2} < TOL$ then
OUTPUT (x); (The procedure was
successful.)
STOP

Step 2.4 If $f(a) \times f(x) > 0$, then set $a = x$; $f(a) = f(x)$ else set $b = x$. (Compute a_i, b_i)

Step 3 OUTPUT ('The method failed after N_0 iterations, $N_0 = , N_0$); (The procedure was unsuccessful.)
STOP.

2. Newton-Raphson's Method

Consider the Taylor Series expansion of $f(x)$ about some point $x = x_0$.

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$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0) + O(|x - x_0|^3). \quad (8)$$

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Subsequent iterations are defined in a similar manner as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad (10)$$

Newton-Raphson's Method

Geometrically, x_{n+1} can be interpreted as the value of x at which a line, passing through the point $(x_n, f(x_n))$ and tangent to the curve $f(x)$ at that point, crosses the y axis. Figure 1 provides a graphical interpretation of this.

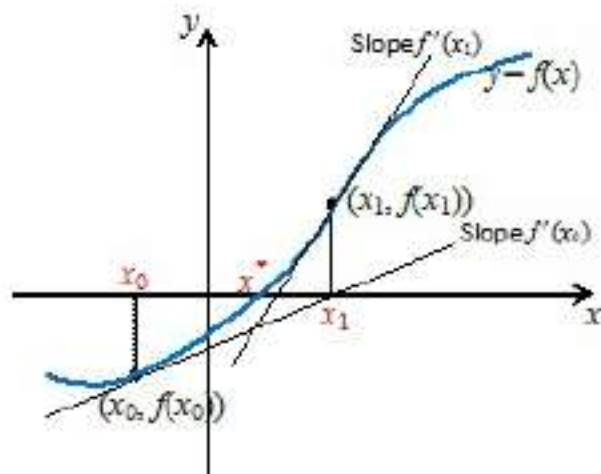


Figure 1: Iterations Newton's method

Example

We use the Newton's method to determine $\sqrt{5}$.

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Solution:

We start with $f(x) = x^2 - A$, observe that the roots of the equation $x^2 - A = 0$ are $\pm\sqrt{A}$. Next use $f(x)$ and its derivative, $f'(x) = 2x$ and also $x_0 = 2$. After simplification, we have

$$x_{n+1} = \frac{x_n + \frac{A}{x_n}}{2}$$

Now, we use equation (10) to solve the problem and we obtain:

$$x_1 = \frac{2 + \frac{5}{2}}{2} = 2.25$$

$$x_2 = \frac{2.25 + \frac{5}{2.25}}{2} = 2.236111111$$

$$x_3 = \frac{2.236111111 + \frac{5}{2.236111111}}{2} = 2.236067978$$

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If we continue for $n > 4$, we will obtain $x_k = 2.236067978$. Hence, we conclude that convergence accurate to nine significant digits has been obtained.

2.1 Convergence

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Suppose that $\{x_n\}_0^\infty$ converges to x^* , and set $e_{n+1} = x_{n+1} - x^*$ for $n \geq 2$. By using Taylor's series expansion around x^* we have

$$e_{n+1} = \frac{1}{2}e_n^2 \frac{f''(x^*)}{f'(x^*)} + O(e_n^3)$$

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$$e_{n+1} = \frac{1}{2}e_n^2 \frac{f''(x^*)}{f'(x^*)} + O(e_n^3)$$

since $f(x^*) = 0$. Thus, by comparison with (4), there is second order (quadratic) convergence. The presence of the f' term in the denominator shows that the scheme will not converge if f' vanishes in the neighborhood of the root.

2.2 Newton's Algorithm

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INPUT: Initial approximation x_0 ; tolerance TOL; maximum number of iterations N_0 .

OUTPUT: approximate solution x^* or message of failure.

Step 1 Set $i = 1$.

Step 2 While $i \leq N_0$ do Step 2.1 - 2.4.

Step 2.1 Set $x = x_0 - \frac{f(x_0)}{f'(x_0)}$. (Compute x_i)

Step 2.2 If $|x - x_0| < TOL$ then
OUTPUT (x); (The procedure was successful.)
STOP

Step 2.3 Set $i = i + 1$.

Step 2.4 Set $x_0 = x$. (Update x_0)

Step 3 UOUTPUT ('The method failed after N_0 iterations, $N_0 = , N_0$); (The procedure was unsuccessful.)
STOP.

2.3 Stopping Criterion

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The stopping-technique inequalities given with the Bisection method are applicable to Newton's method. That is, select a tolerance $\epsilon > 0$, and construct x_1, x_2, \dots, x_n , until

$$|x_n - x_{n-1}| < \epsilon, \quad (11)$$

$$\frac{|x_n - x_{n+1}|}{|x_n|} < \epsilon, \quad x_n \neq 0, \quad (12)$$

or

$$|f(x_n)| < \epsilon. \quad (13)$$

Ordinary Differential Equations

1. Euler's Method

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The basic idea of differential calculus at the any point is that a function value and its tangent line do not differ very much. Consider, for example, the function $f(x) = \cos x$ and its tangent line at $\frac{\pi}{3}$. Figure 2 provides a graphical interpretation of this

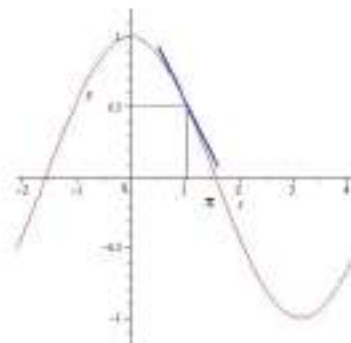


Figure 2: Tangent line

Now, consider the differential equation

$$\frac{dy}{dx} = x - y \quad (14)$$

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If we want to compute the solution passing through the point $(-1, 4)$, then we can compute the tangent line at this point. It's slope at $x = -1$ is given by the differential equation

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$$y'(-1) = -1 - 4 = -5. \quad (15)$$

Thus the equation for the tangent line

$$y(x) = 4 - 5(x + 1) \quad (16)$$

Since we expect the solution to the differential equation and its tangent line to be close when x is close to -1 . We should also expect that the solution to the differential equation at, let's say $x = -0.75$ will be closed to the tangent line at $x = -0.75$.

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The y -value of the tangent line is

$$\begin{aligned}y(-0.75) &= 4 - 5(-0.75 + 1) \\ &= 2.75\end{aligned}$$

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The y -value of the tangent line is

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The tangent line equation for $x = -0.75$ and $y = 2.75$ is given by

$$y(x) = 2.75 - 3.5(x + 0.75)$$

Euler's Method

By using the tangent line equation for $x = -0.5$ we obtain

$$\begin{aligned}y(-0.5) &= 2.75 - 3.5(-0.5 + 0.75) \\ &= 1.875.\end{aligned}$$

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And if we continued the process, we can obtain the solution of (13) approximately. The graph of tangent line is given in Figure 3 below.

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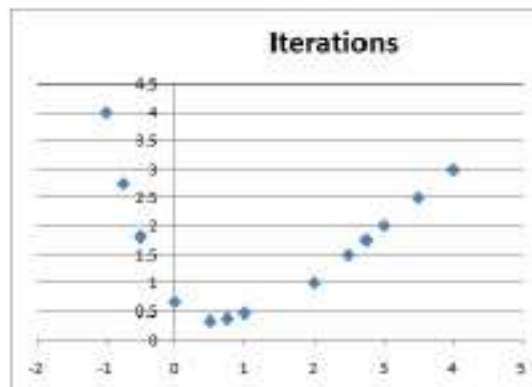


Figure 3: Iteration of Euler's method

Euler's Method

The procedure of Euler's method is given below:

Start at the point (x_0, y_0) , let h denote the x -increment. Then $x_1 = x_0 + h$, where y_1 is the y -coordinate of the point on the line passing through (x_0, y_0) with slope $y'(x_0) = f(x_0, y_0)$. Thus

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The next approximation is found by replacing x_0 and y_0 by x_1 and y_1 . So,

$$x_2 = x_1 + h \quad \text{and} \quad y_2 = y_1 + hf(x_1, y_1)$$

$$\vdots = \vdots \quad \quad \quad \vdots$$

$$x_k = x_{k-1} + h \quad \text{and} \quad y_k = y_{k-1} + hf(x_{k-1}, y_{k-1}).$$

In general, we obtain the following formula for $n = 1, 2, 3, \dots$

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In general, we obtain the following formula for $n = 1, 2, 3, \dots$

$$x_n = x_{n-1} + h \quad \text{and} \quad y_n = y_{n-1} + hf(x_{n-1}, y_{n-1}).$$

We obtain the better approximation if we reduce the step size h .

The following graph give approximations for step size $h = 0.25$, $h = 0.1$ and $h = 0.01$.

For this example it is not hard to compute the exact solution

$$y = -1 + 6e^{-(1+x)}.$$

Euler's Method

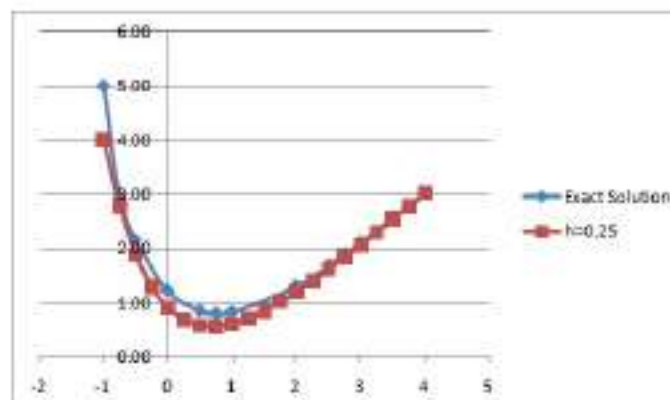


Figure: Exact solution vs Approximate solution with $h = 0.25$

Euler's Method

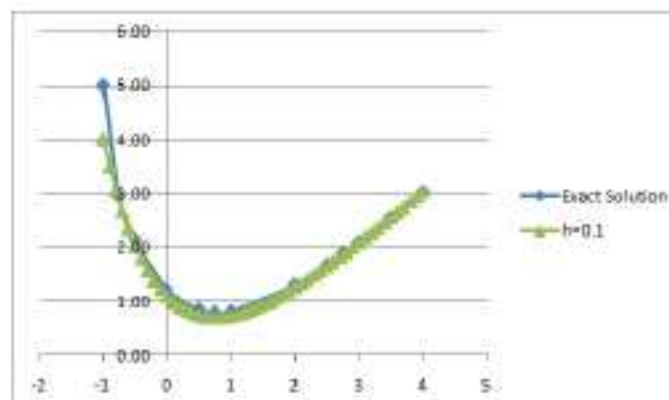


Figure: Exact solution vs Approximate solution with $h = 0.1$

Euler's Method

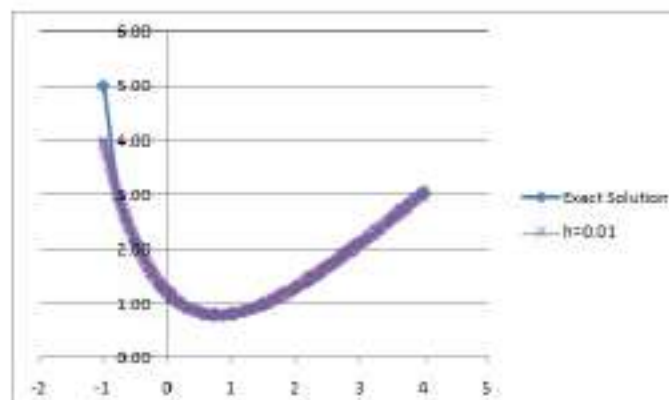


Figure: Exact solution vs Approximate solution with $h = 0.01$

1.2 Euler's Algorithm

To approximate the solution of initial-value problem

$$y' = f(x, t), \quad a \leq t \leq b, \quad y(a) = \alpha$$

at $(N + 1)$ equally spaced numbers in the interval $[a, b]$.

INPUT: Endpoints a and b ; Integer N ; Initial condition α .

OUTPUT: Approximation w to y at the $(N + 1)$ values of t .

Step 1 Set $h = \frac{b-a}{N}$; $t = a$; $w = \alpha$

OUTPUT (t, w)

Step 2 For $i = 1, 2, \dots, N$ do Step 2.1-2.2

Step 2.1 Set $w = w + hf(t, w)$; Compute w ;

$t = a + ih$ Compute t ;

Step 2.2 OUTPUT (t, w) .

Step 3 STOP

1. Practical Harmonic Analysis

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- 1 Engineers often deal with systems that oscillate or vibrate.
- 2 Therefore trigonometric functions play a fundamental role in modeling such problems.
- 3 Fourier approximation represents a systemic framework for using trigonometric series for this purpose.

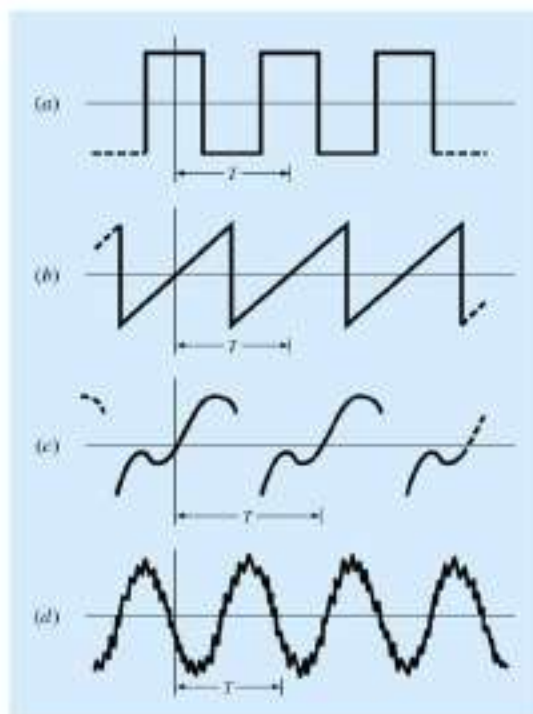


Figure: (a) The square wave, (b) The sawtooth wave, (c) Non ideal (d) contaminated by noise

- A periodic function $f(t)$ is one for which $f(t) = f(t + L)$, where T is a constant called the period that is the smallest value for which this equation holds.
- Any waveform that can be described as a sine or cosine is called sinusoid:

$$f(t) = A_0 + C_1 \cos(\omega_0 t + \theta)$$

Four parameters serve to characterize the sinusoid:

- The mean value A_0 sets the average height above the abscissa.
- The amplitude C_1 specifies the height of the oscillation.
- The angular frequency ω_0 characterizes how often the cycles occur.
- The phase angle, or phase shift, θ parameterizes the extent which the sinusoid is shifted horizontally.

1.1 Least-Squares Fit of a Sinusoid

- Sinusoid equation can be thought of as a linear least-squares model

$$y = A_0 + A_1 \cos(\omega_0 t) + B_1 \sin(\omega_0 t) + e$$

- Thus our goal is to determine coefficient values that minimize

$$S_r = \sum_{i=1}^N \{y_i - (A_0 + A_1 \cos(\omega_0 t_i) + B_1 \sin(\omega_0 t_i))\}^2$$

Where the coefficients can be determined as

$$A_0 = \frac{\sum y}{N}$$

$$A_1 = \frac{2}{N} \sum y \cos(\omega_0 t)$$

$$B_1 = \frac{2}{N} \sum y \sin(\omega_0 t)$$

Example

The curve in Figure below is described by $y = 1.7 + \cos(4.189t + 1.0472)$. Generate 10 discrete values for this curve at intervals of $\Delta t = 0.15$ for the range $t = 0$ to 1.35. Use this information to evaluate the coefficients of A_0, A_1, B_1 by least squares fit.

Fourier Series

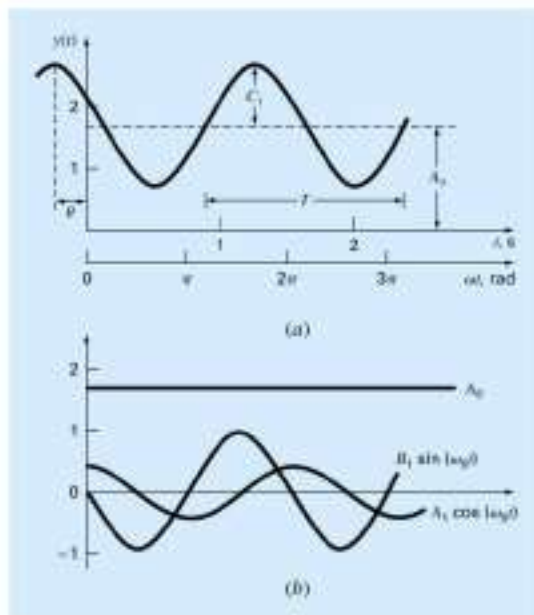


Figure: A plot of the sinusoidal $y(t) = A_0 + C_1 \cos(\omega_0 t + \theta)$

The data required to evaluate the coefficients with $\omega = 4.189$ are

t	y	$y \cos(\omega t)$	$y \sin(\omega t)$
0.00	2.200	2.200	0.000
0.15	1.595	1.290	0.938
0.30	1.031	0.319	0.981
0.45	0.722	-0.223	0.687
0.60	0.786	-0.636	0.462
0.75	1.200	-1.200	0.000
0.90	1.805	-1.460	-1.061
1.05	2.369	-0.732	-2.253
1.20	2.678	0.828	-2.547
1.35	2.614	2.115	-1.536
Sum	17.000	2.502	-4.331

Figure: data

For this case $A_0 = \frac{17.000}{10} = 1.7$, $A_1 = \frac{2}{10}(2.502) = 0.500$ and $B_1 = \frac{2}{10}(-4.330) = -0.866$

Thus, the least-squares fit is

$$y = 1.7 + 0.500 \cos(\omega_0 t) - 0.866 \sin(\omega_0 t)$$

The model can also be express by

$$y = 1.7 + \cos(\omega_0 t + 1.0472)$$

where

$$\theta = \arctan\left(-\frac{-0.866}{0.500}\right) = 1.0472,$$
$$C_1 = \sqrt{(0.5)^2 + (-0.866)^2} = 1.00$$

1.2 Continuous Fourier Series

Harmonic Analysis is the theory of expanding a given function in Fourier series.

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Divide the interval $[-\pi, \pi]$ into n equal parts with $(n + 1)$ points

$$-\pi = x_0, x_1, x_2, \dots, x_n = \pi$$

and subinterval size $h = \frac{2\pi}{n}$

Let $y_i = f(x_i)$, for $i = 0, 1, 2, \dots, n$.

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Then the Fourier coefficients (17) - (19) are determined approximately by the following:

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx = \frac{1}{\pi} \left(\sum_{i=1}^n h \cdot y_i \right) = \frac{1}{\pi} \cdot \frac{2\pi}{n} \sum_{i=1}^n y_i$$

or

$$a_0 = \frac{2}{\pi} \sum_{i=1}^n y_i \quad (20)$$

Also

$$\begin{aligned} a_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx = \frac{1}{\pi} \left(\sum_{i=1}^n h \cdot y_i \cos nx_i \right) \\ &= \frac{1}{\pi} \cdot \frac{2\pi}{n} \sum_{i=1}^n y_i \cos nx_i. \end{aligned}$$

or,

$$a_n = \frac{2}{\pi} \sum_{i=1}^n y_i \cos nx_i. \quad (21)$$

Similarly,

$$b_n = \frac{2}{\pi} \sum_{i=1}^n y_i \sin nx_i. \quad (22)$$

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Note: Choose n as a number divisibly by 4 since the values of **sine** and **cosine** are repeated in four quadrants. Usually, choice $n = 6, 12, 24$ (in which case (20), (21) and (22) get simplified).

Example

Compute approximately the Fourier coefficients a_0, a_1, a_2, a_3 and b_1, b_2, b_3 in the Fourier series expansion of function tabulated as follows. Find the amplitude and the first harmonic. Calculate $y(3)$.

x :	0	1	2	3	4	5
y :	9	18	24	28	26	20

Solution:

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Solution:

The number of sub interval (n) = 6. The interval $(0, 2\pi)$ is divided into 6 sub-intervals of size $\frac{2\pi}{6} = 60^\circ$.

Table 1.1

x	θ	$\cos \theta$	$\cos 2\theta$	$\cos 3\theta$	y	$y \cos \theta$	$y \cos 2\theta$	$y \cos 3\theta$
0	0°	1	1	1	9	9	9	9
1	60°	$+1/2$	$-1/2$	-1	18	-9	-9	-18
2	120°	$-1/2$	$-1/2$	1	24	-12	-12	24
3	180°	-1	+1	-1	28	-28	28	-28
4	240°	$-1/2$	$-1/2$	1	26	-13	-13	26
5	300°	$+1/2$	$-1/2$	-1	20	10	-10	-20
				Σ	125	-25	-7	-7

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$$a_2 = \frac{2}{n} \sum_{i=1}^n y_i \cos 2x_i = \frac{2}{6}(-7) = -2.333$$

$$a_3 = \frac{2}{n} \sum_{i=1}^n y_i \cos 3x_i = \frac{2}{6}(-7) = -2.333$$

Similarly,

Table 1.2

x	θ	$\sin \theta$	$\sin 2\theta$	$\sin 3\theta$	y	$y \sin \theta$	$y \sin 2\theta$	$y \sin 3\theta$
0	0°	0	0	0	9	0	0	0
1	60°	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	18	$9\sqrt{3}$	$9\sqrt{3}$	0
2	120°	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	24	$12\sqrt{3}$	$-12\sqrt{3}$	0
3	180°	0	0	0	28	0	0	0
4	240°	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$	0	26	$-13\frac{\sqrt{3}}{2}$	$13\frac{\sqrt{3}}{2}$	0
5	300°	$-\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	20	$-10\frac{\sqrt{3}}{2}$	$-10\frac{\sqrt{3}}{2}$	0
				Σ	125	$-2\sqrt{3}$	0	0

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$$b_1 = \frac{2}{n} \sum_{i=1}^n y_i \sin x_i = \frac{2}{6}(-2\sqrt{3}) = -1.1547$$

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$$b_3 = 0.$$

Amplitude of the first harmonic

$$= \sqrt{a_1^2 + b_1^2} = \sqrt{(-8.333)^2 + (-1.1547)^2} = 8.4126.$$

Fourier Series

The Fourier series of $y(x)$ containing the first 4 cosine terms and 3 sine terms is

$$y = \frac{41.666}{2} + (-8.333) \cos x - 2.333 \cos 2x + (-2.333) \cos 3x + (-1.1547) \sin x + 0 + 0$$

At $x = 3$, $\theta = \pi$

$$\begin{aligned} y(3) = y(\pi) &= \frac{41.666}{2} + (-8.333)(-1) - 2.333(1) - \\ &= (-2.333)(-1) - 1.1547(0) = 29.166 \end{aligned}$$

The exact value $y(3) = 28$

The Graph of the Data and Fourier series expansion is given on the next figure.

Table 1.3: Fourier Series

x	y	theta	\tilde{y}
0	9	0.00	7.830
1	18	1.05	19.171
2	24	2.09	22.830
3	28	3.14	29.170
4	26	4.19	24.828
5	20	0.00	7.830

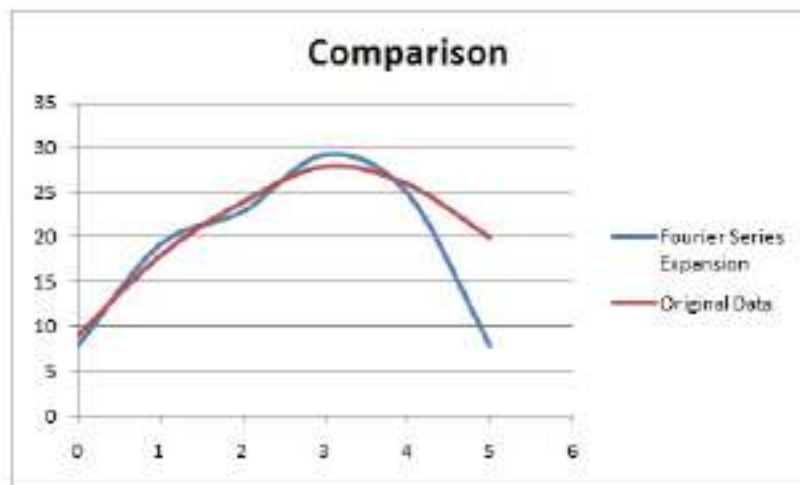


Figure: of the Fourier

Partial Differential Equation

An equation involving partial derivatives of an unknown function of two or more independent variables.

General form of PDE

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$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial y \partial x} + C \frac{\partial^2 u}{\partial y^2} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + F u(x, y) + G = 0$$

Could be classified into 3 types: **parabolic**, **hyperbolic** and **elliptic**, depending on the sign of $B^2 - 4AC$.

If $B^2 - 4AC = 0 \rightarrow$ parabolic

Example

Heat equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{1}{k} \frac{\partial u}{\partial t} = 0$$

If $B^2 - 4AC > 0 \rightarrow$ hyperbolic

Example

Wave equation:

$$\frac{\partial^2 u}{\partial x^2} - a^2 \frac{\partial^2 u}{\partial y^2} = 0$$

If $B^2 - 4AC = 0 \rightarrow$ elliptic

Example

Laplace's equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + u(x, y) = 1$$

To solve, we use the **finite-difference methods** as follows:

1st Step Choose n and m , and define

$$h = \frac{a - b}{n}, \quad k = \frac{c - d}{m}$$

→ Partition $[a, b]$ into n equal parts of width h and $[c, d]$ into m equal parts of width k .

→ Place a grid on the rectangular R by drawing vertical & horizontal lines through the points with coordinates (x_i, y_j) , where

$$x_i = a + ih, \quad y_j = c + jk, \quad (i = 0, 1, \dots, n; j = 0, 1, \dots, m).$$

→ The line $x = x_i$ and $y = y_j$ are **grid lines** and their intersections are the **mesh points** of the grid.

2nd Step For each mesh points in the interior of the grid $(x_i, y_j), (i = 1, 2, \dots, n - 1; j = 1, 2, \dots, m - 1)$, we use Taylor's series to generate the **finite-difference formula**.

- The forward-difference formula for $u_t(x, y)$ & $u_x(x, t)$:

$$\left(\frac{\partial u}{\partial t}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{k}, \quad \left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{h}.$$

- Centered-difference formula for $u_t(x, y)$ & $u_x(x, t)$:

$$\left(\frac{\partial u}{\partial t}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2k}, \quad \left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h}$$

- The backward-difference formula for $u_t(x, y)$ & $u_x(x, t)$:

$$\left(\frac{\partial u}{\partial t}\right)_{ij} = \frac{u_{ij} - u_{i,j-1}}{k}, \quad \left(\frac{\partial u}{\partial x}\right)_{ij} = \frac{u_{ij} - u_{i-1,j}}{h}$$

- Centered-difference formula for $u_{tt}(x, y)$ & $u_{xx}(x, t)$:

$$\left(\frac{\partial^2 u}{\partial t^2}\right)_{ij} = \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{k^2},$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ij} = \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2}$$

The resulting system equations can be solved by Gauss-Seidel method.

Example & Exercise (Partial Differential Equations)

Thanks