Introduction to Scientific Computing

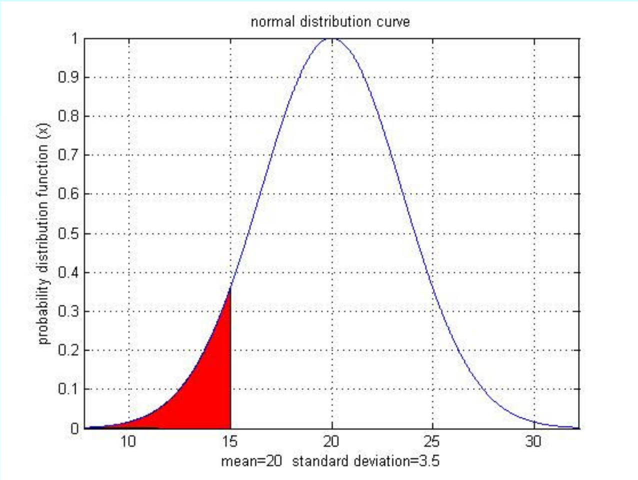
Author: Autar Kaw, Luke Snyder

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Why use Numerical Methods?

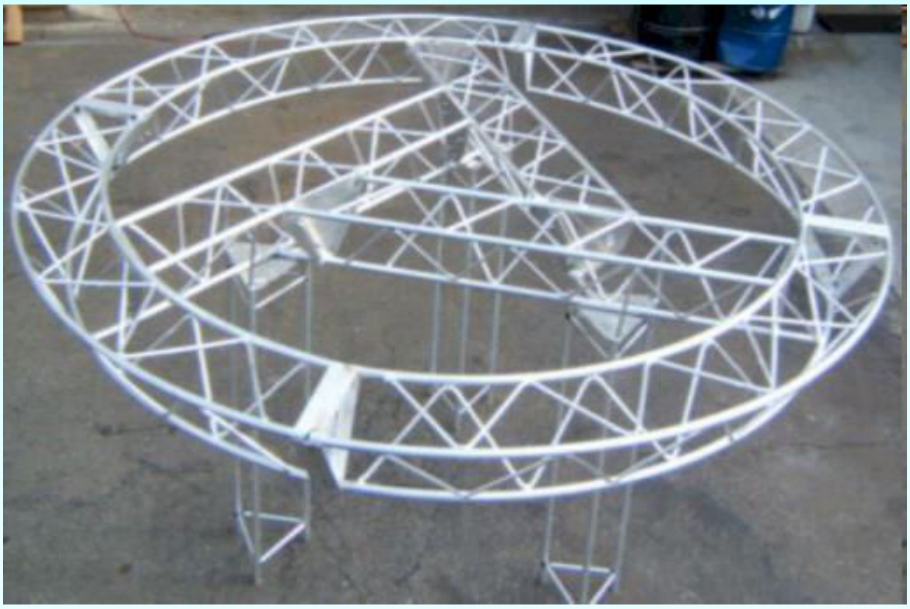
- To solve problems that cannot be solved exactly

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} e^{-\frac{u^2}{2}}\,du$$



Why use Numerical Methods?

- To solve problems that are intractable!
  - No efficient algorithm is available



Steps in Solving an Engineering Problem

How do we solve an engineering problem?

Problem Description

↓

Mathematical Model

↓

Solution of Mathematical Model

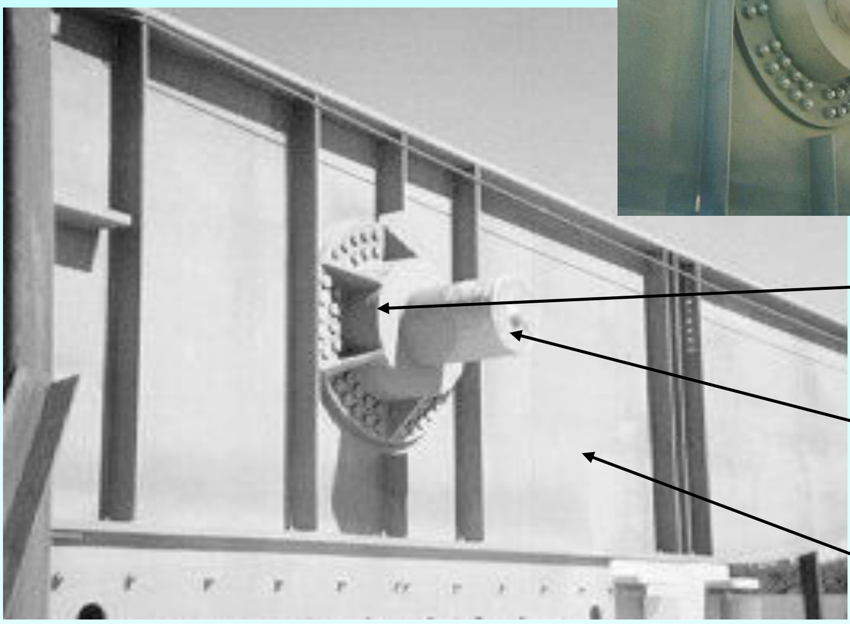
↓

Using the Solution

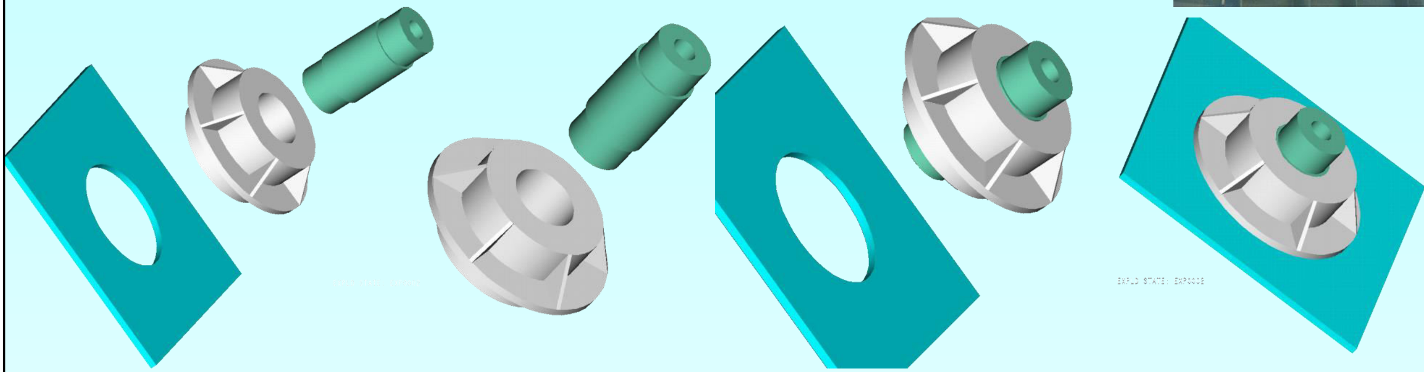
Example of Solving an Engineering Problem

Bascule Bridge THG

Bascule Bridge THG



Trunnion-Hub-Girder Assembly Procedure



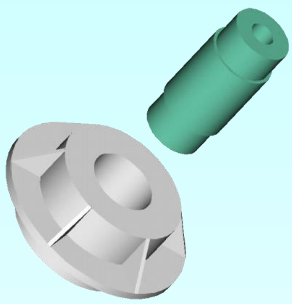
Step1. Trunnion immersed in dry-ice/alcohol

Step2. Trunnion warm-up in hub

Step3. Trunnion-Hub immersed in dry-ice/alcohol

Step4. Trunnion-Hub warm-up into girder

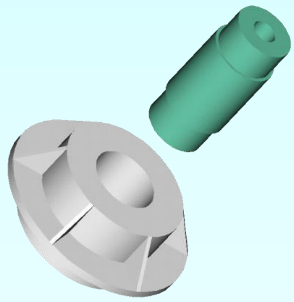
Problem



After Cooling, the Trunnion Got Stuck in Hub

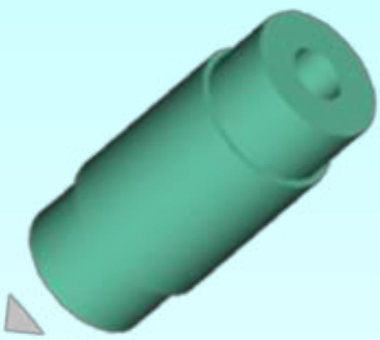
Why did it get stuck?

Magnitude of contraction needed in the trunnion was 0.015” or more. Did it contract enough?



Consultant calculations

$$\Delta D = D \times \alpha \times \Delta T$$



$$D = 12.363''$$

$$\alpha = 6.47 \times 10^{-6} in / in /^{o} F$$

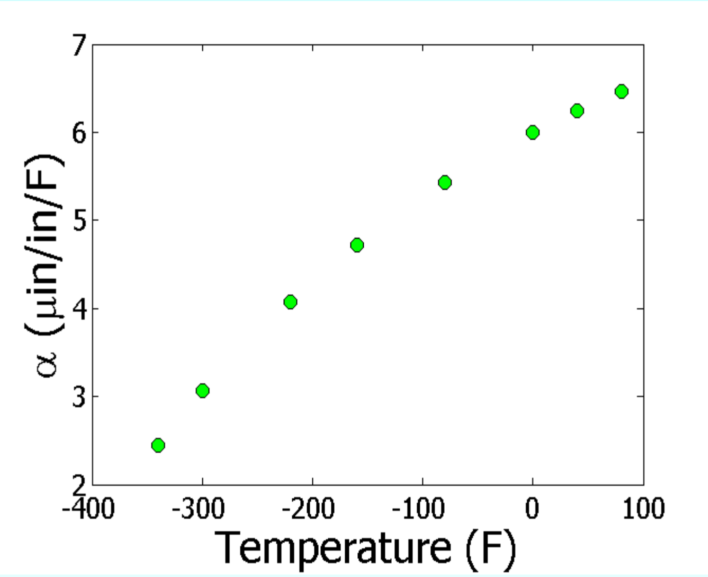
$$\Delta T = -108 - 80 = -188^{o} F$$

$$\Delta D = (12.363)(6.47 \times 10^{-6})(-188)$$

$$= -0.01504''$$

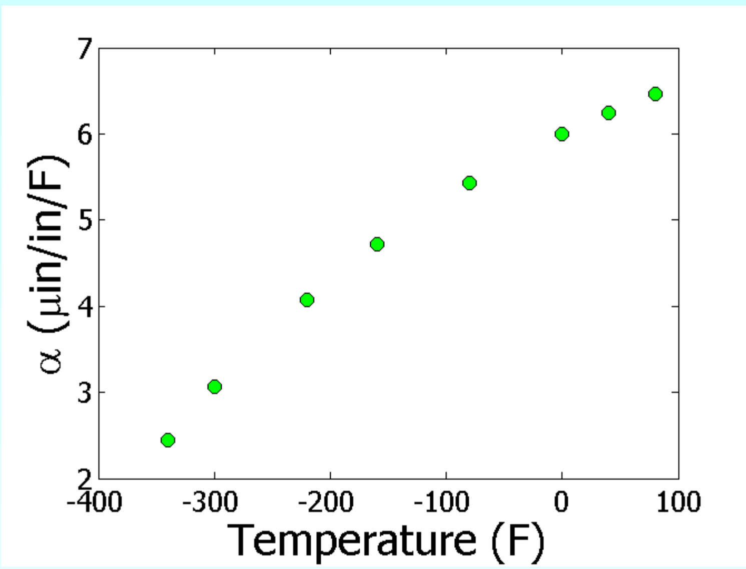
Is the formula used correct?

$$\Delta D = D \times \alpha \times \Delta T$$



T(°F)	α (μin/in/°F)
-340	2.45
-300	3.07
-220	4.08
-160	4.72
-80	5.43
0	6.00
40	6.24
80	6.47

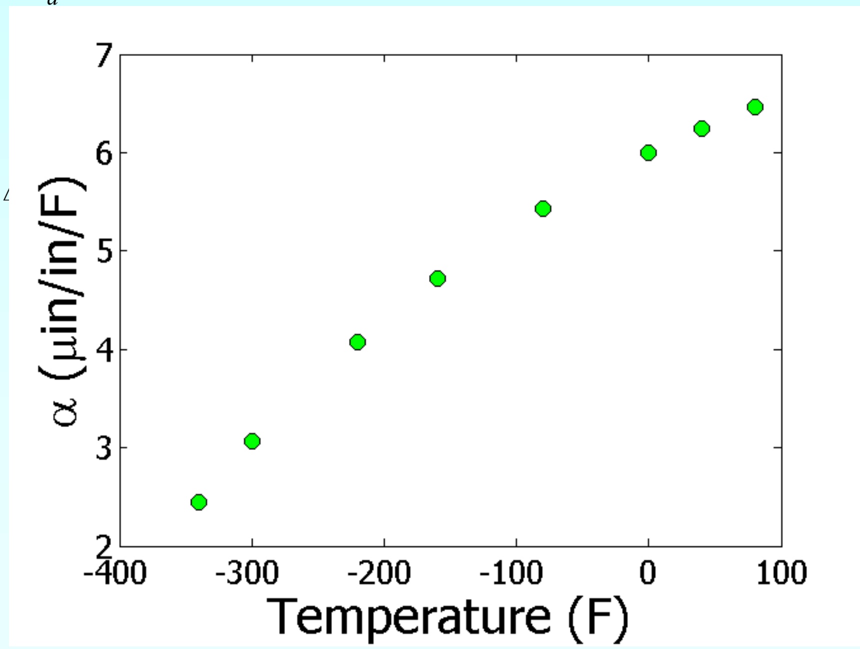
The Correct Model Would Account for Varying Thermal Expansion Coefficient



$$\Delta D = D \int_{T_a}^{T_c} \alpha(T)\,dT$$

Can You Roughly Estimate the Contraction?

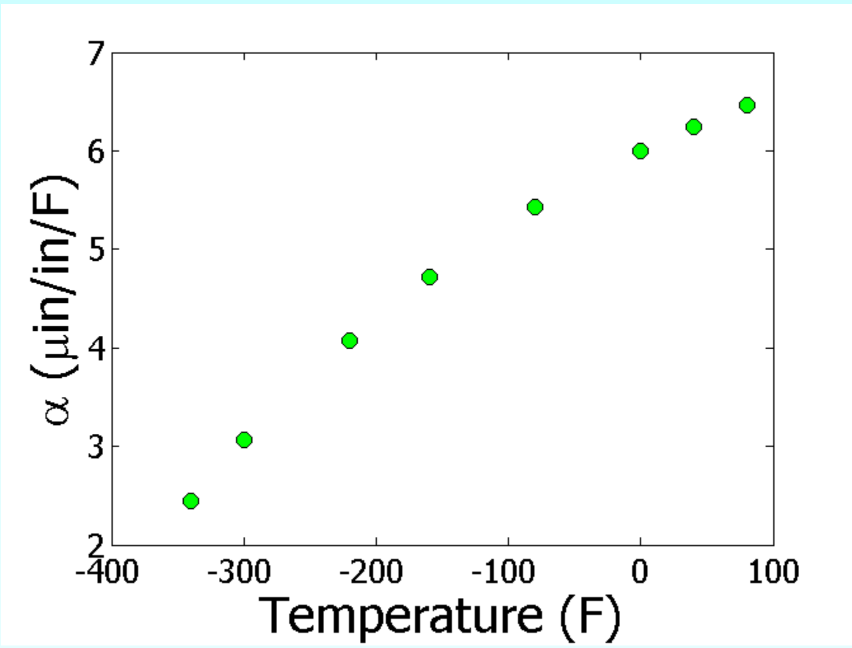
$$\Delta D = D\int_{T_a}^{T_c} \alpha(T)dT$$ T_a=80°F; T_c=-108°F; D=12.363″



Can You Find a Better Estimate for the Contraction?

$$\Delta D = D\int_{T_a}^{T_c} \alpha(T)dT$$

$T_a = 80^oF$
$T_c = -108^oF$
$D = 12.363"$

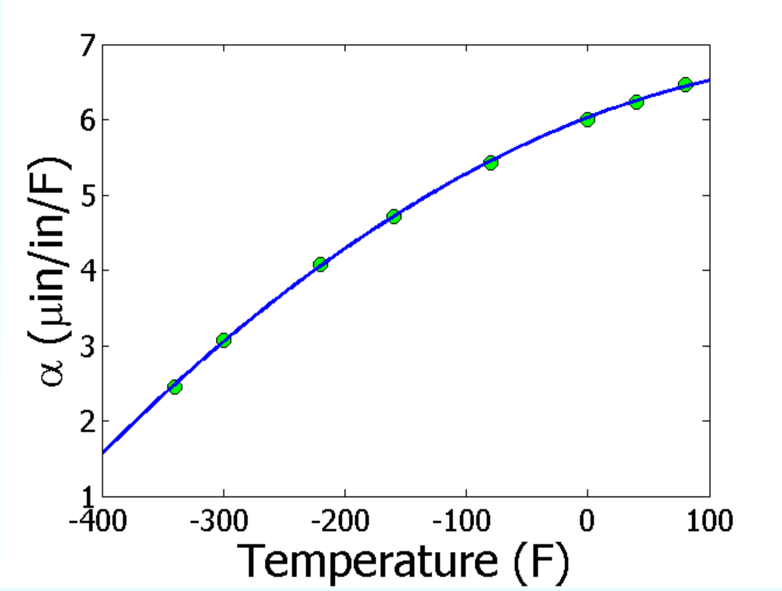


Estimating Contraction Accurately

Change in diameter (ΔD) by cooling it in dry ice/alcohol is given by

$$\Delta D = D\int_{T_a}^{T_c} \alpha(T)dT$$

$T_a = 80^oF$
$T_c = -108^oF$
$D = 12.363''$



$$\alpha = -1.2278\times10^{-5}T^2 + 6.1946\times10^{-3}T + 6.0150$$

$$\Delta D = -0.0137''$$

So what is the solution to the problem?

One solution is to immerse the trunnion in liquid nitrogen which has a boiling point of -321^{o}F as opposed to the dry-ice/alcohol temperature of -108^{o}F.

$$\Delta D = -0.0244''$$

Revisiting steps to solve a problem

1) Problem Statement: Trunnion got stuck in the hub.

2) Modeling: Developed a new model

$$\Delta D = D\int_{T_a}^{T_c} \alpha(T)\,dT$$

3) Solution: 1) Used trapezoidal rule OR b) Used regression and integration.

4) Implementation: Cool the trunnion in liquid nitrogen.

Numerical Methods Application
to
Mathematical Procedures

Mathematical Procedures

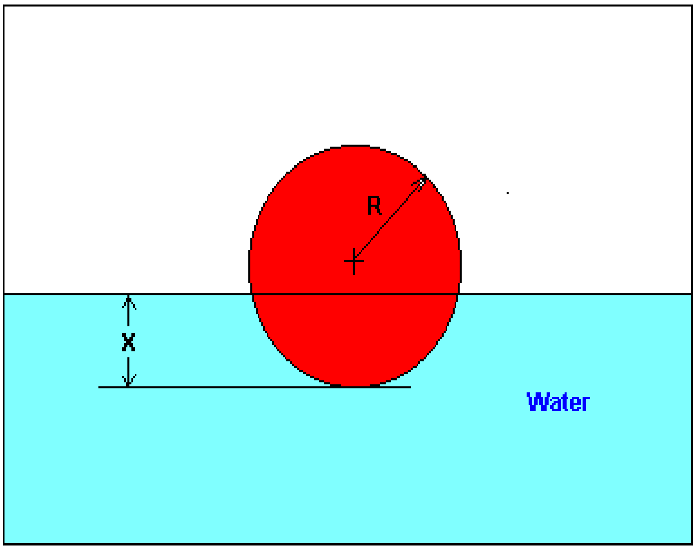
- Nonlinear Equations
- Simultaneous Linear Equations
- Differentiation
- Curve Fitting
  - Interpolation
  - Regression
- Integration
- Ordinary Differential Equations
- Other Advanced Mathematical Procedures:
  - Partial Differential Equations
  - Optimization
  - Fast Fourier Transforms

Nonlinear Equations

How much of the floating ball is under water?

Diameter=0.11m

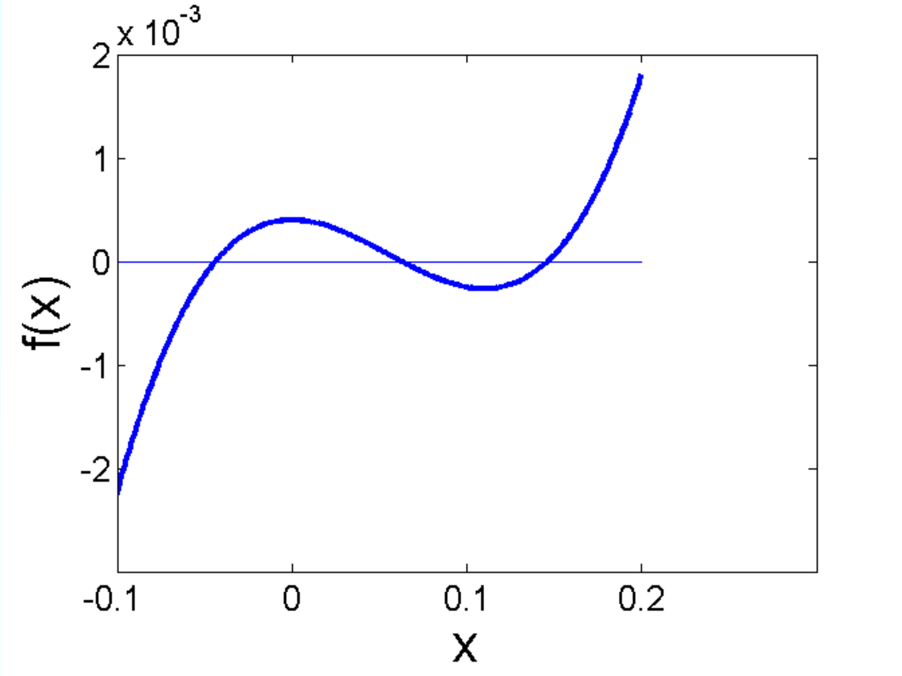
Specific Gravity=0.6



$$x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$$

Nonlinear Equations

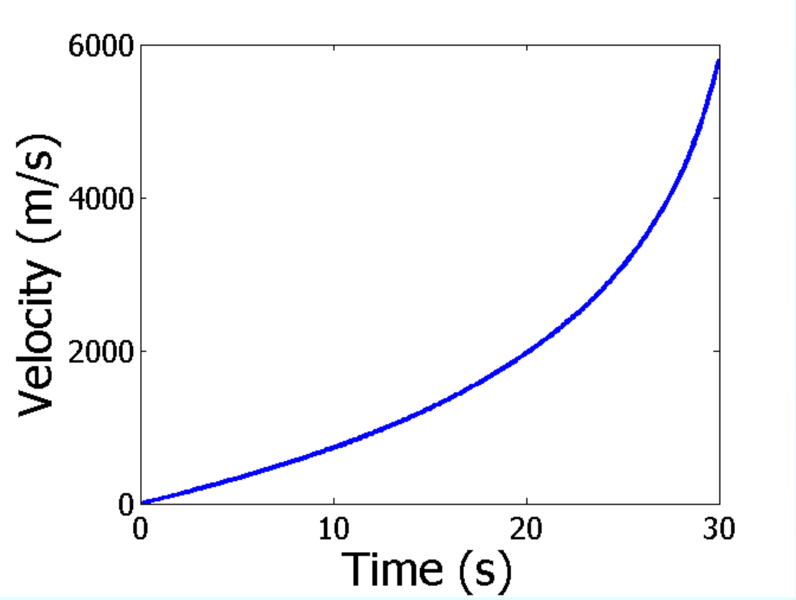
How much of the floating ball is under the water?



$$f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$$

Differentiation

What is the acceleration at t=7 seconds?



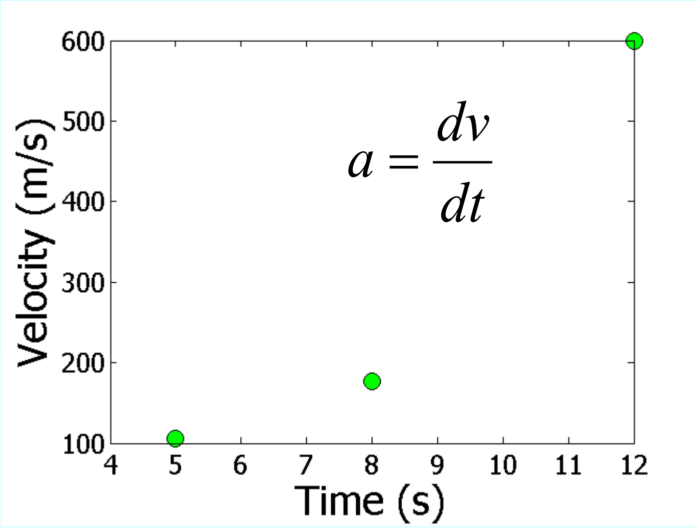
$$v(t) = 2200 \ln\left(\frac{16 \times 10^4}{16 \times 10^4 - 5000t}\right) - 9.8t$$

$$a = \frac{dv}{dt}$$

Differentiation

What is the acceleration at t=7 seconds?

Time (s)	5	8	12
Vel (m/s)	106	177	600



$$a = \frac{dv}{dt}$$

Simultaneous Linear Equations

Find the velocity profile, given

Time (s)	5	8	12
Vel (m/s)	106	177	600

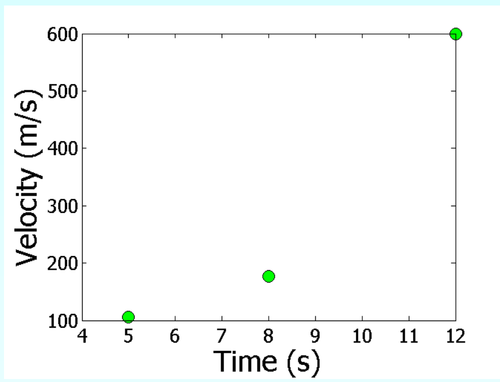
$$v(t) = at^2 + bt + c, \; 5 \le t \le 12$$

Three simultaneous linear equations

$$25a + 5b + c = 106$$

$$64a + 8b + c = 177$$

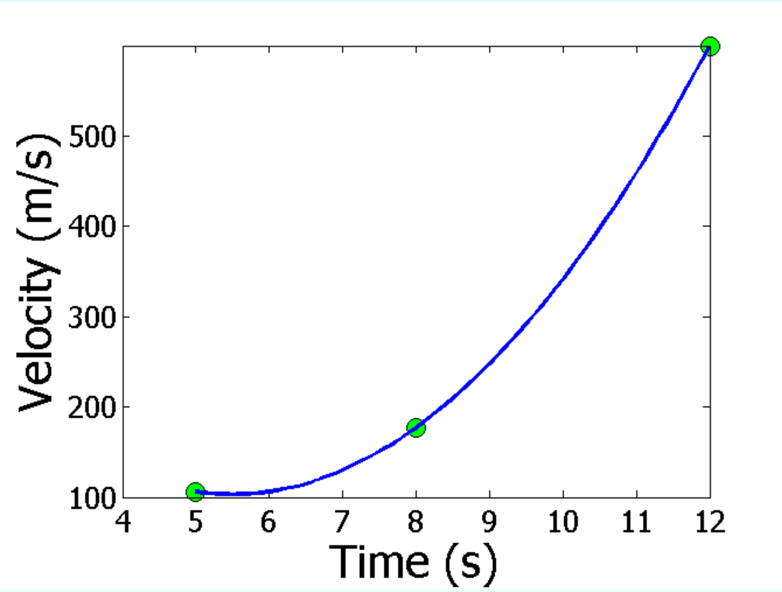
$$144a + 12b + c = 600$$



Interpolation

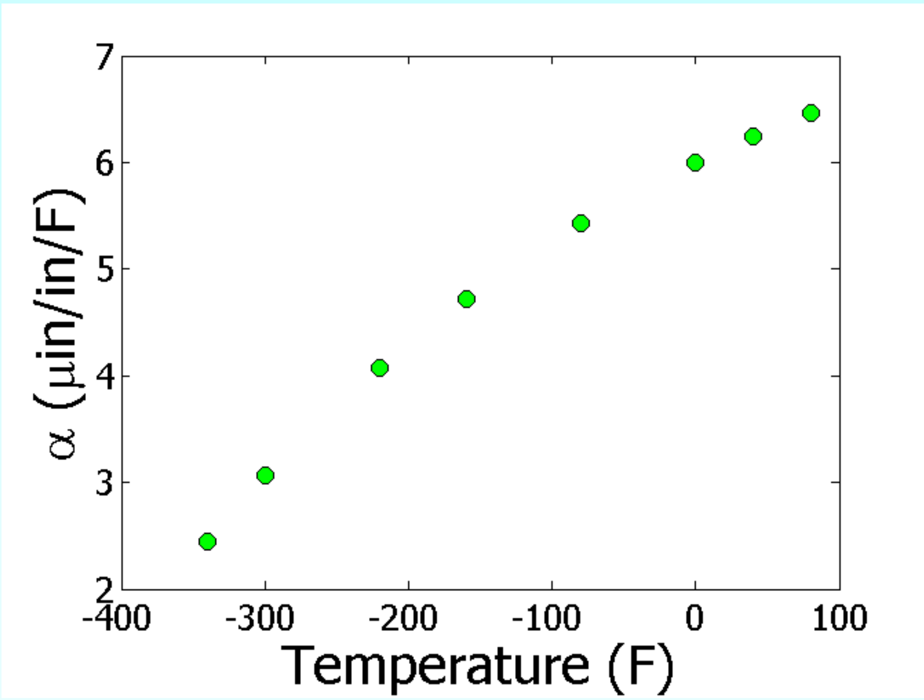
What is the velocity of the rocket at t=7 seconds?

Time (s)	5	8	12
Vel (m/s)	106	177	600

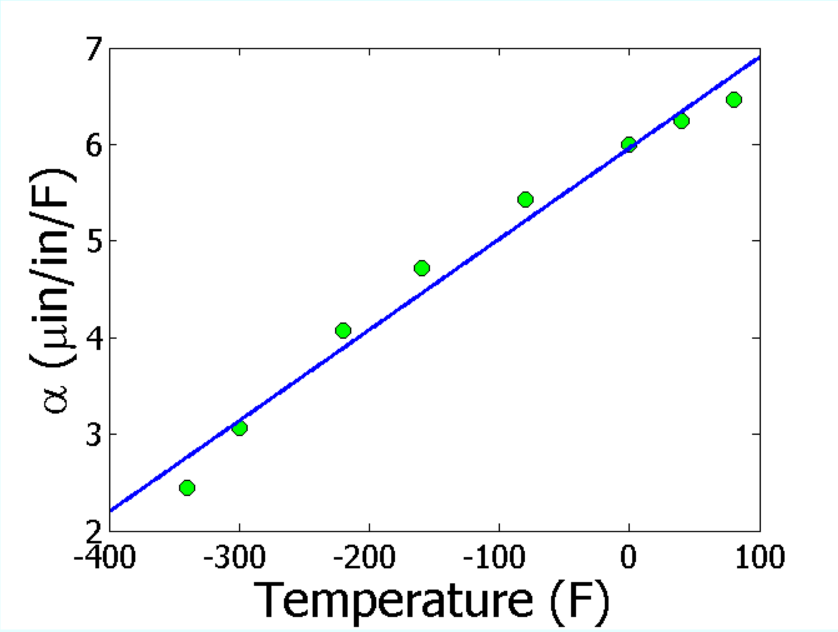


Regression

Thermal expansion coefficient data for cast steel



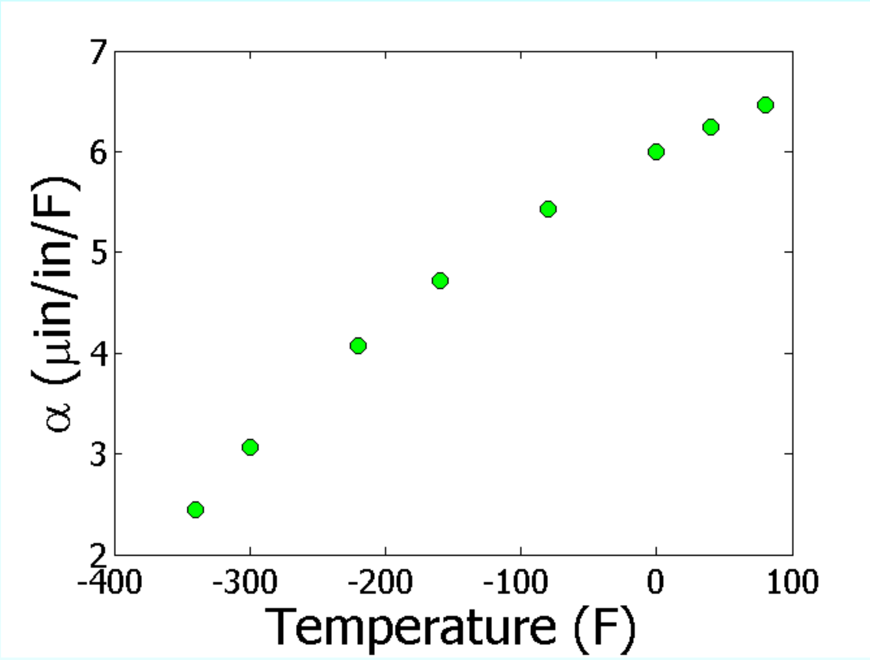
Regression (cont)



Integration

Finding the diametric contraction in a steel shaft when dipped in liquid nitrogen.

$$\Delta D = D \int_{T_{room}}^{T_{fluid}} \alpha \, dT$$



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Introduction to Numerical Methods

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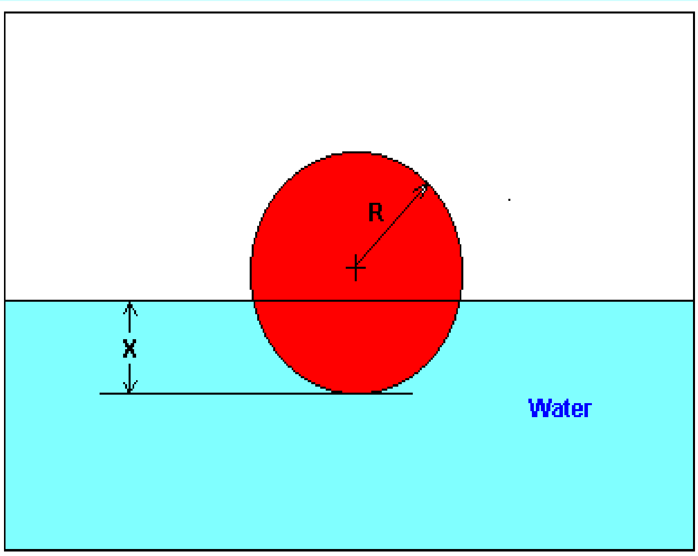
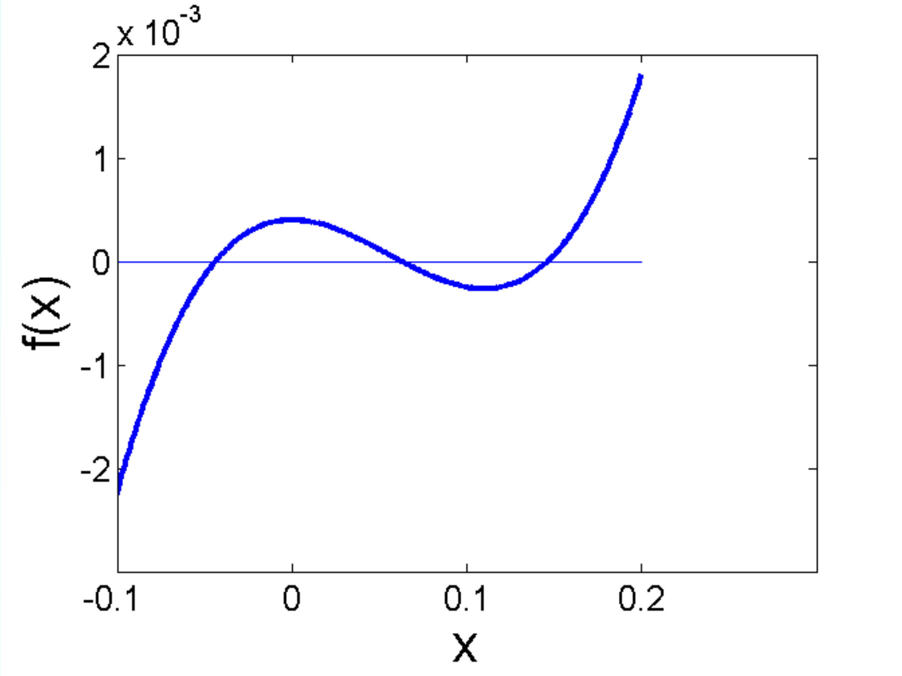


$$x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$$

Nonlinear Equations

How much of the floating ball is under the water?



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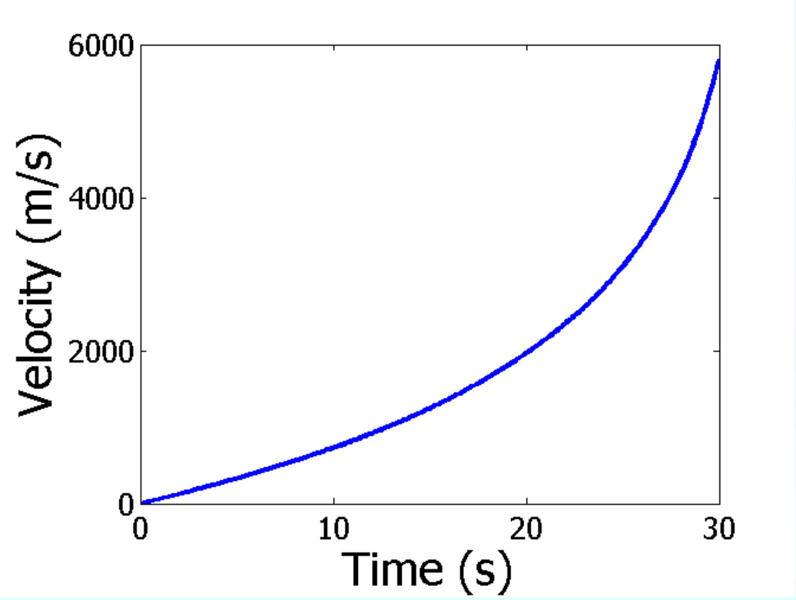

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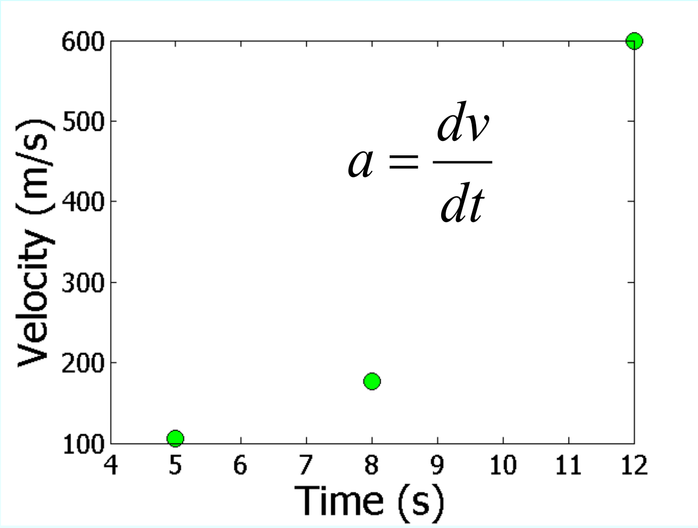

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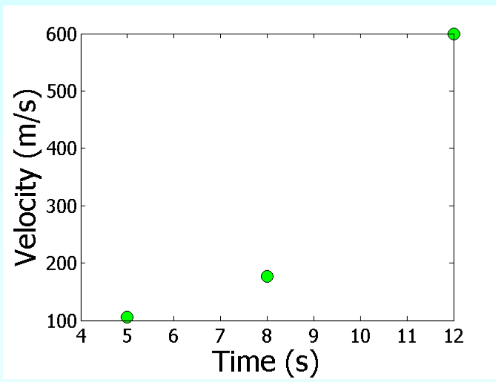

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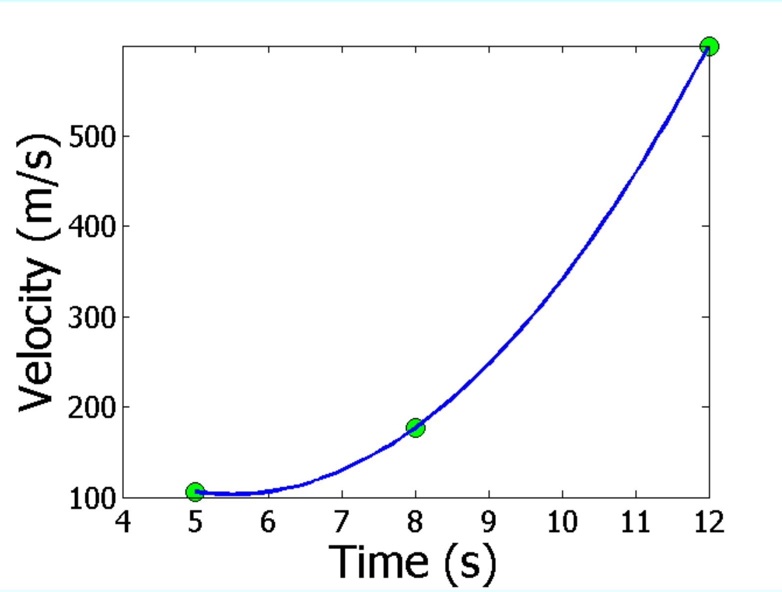

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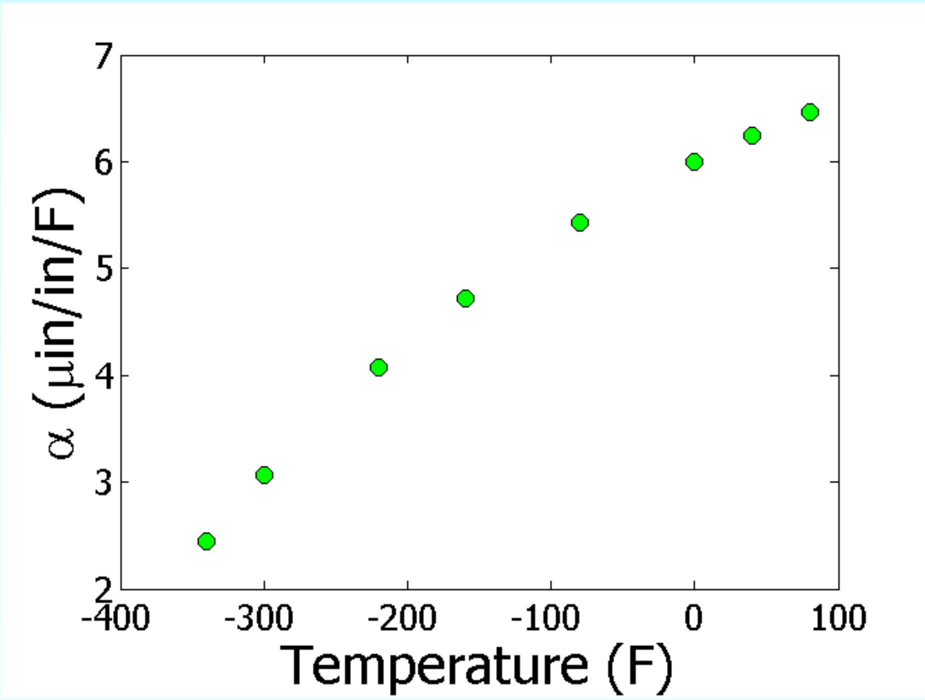
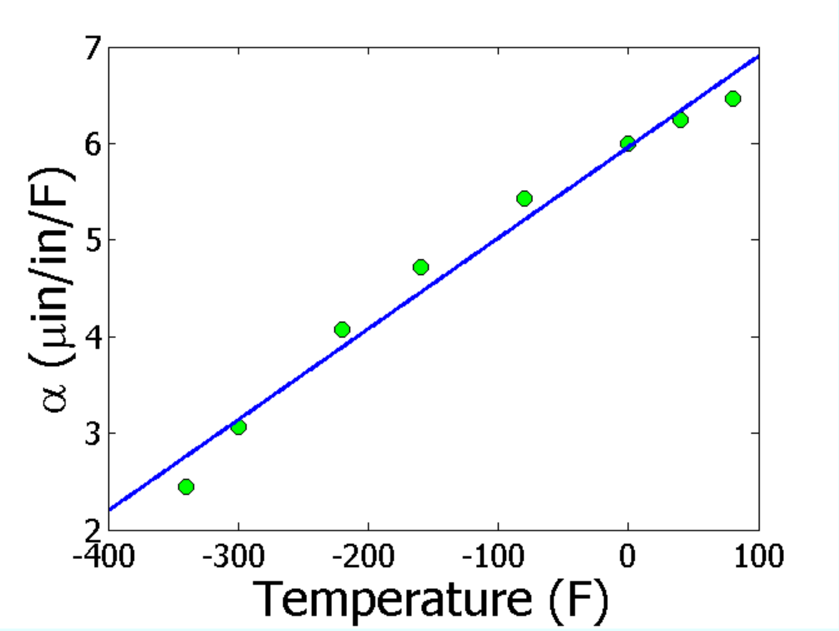


Regression (cont)



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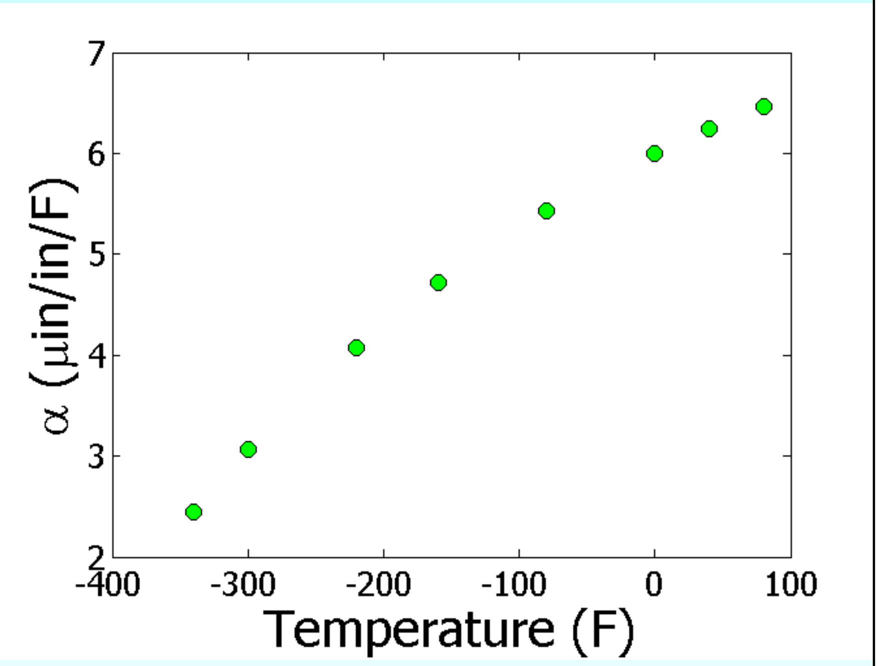

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Solving Nonlinear Equations

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Bisection Method

Basis of Bisection Method

Theorem An equation f(x)=0, where f(x) is a real continuous function, has at least one root between x_l and x_u if $f(x_l)\, f(x_u) < 0$.

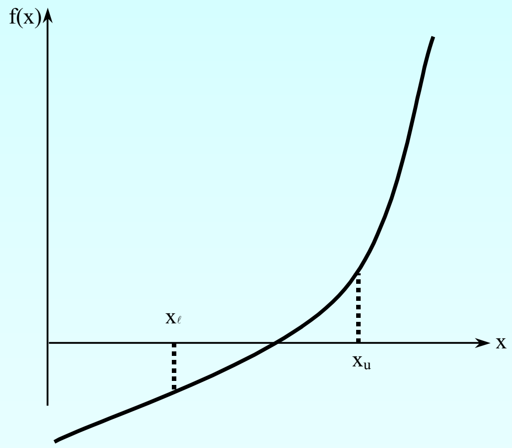


Figure 1 At least one root exists between the two points if the function is real, continuous, and changes sign.

Basis of Bisection Method

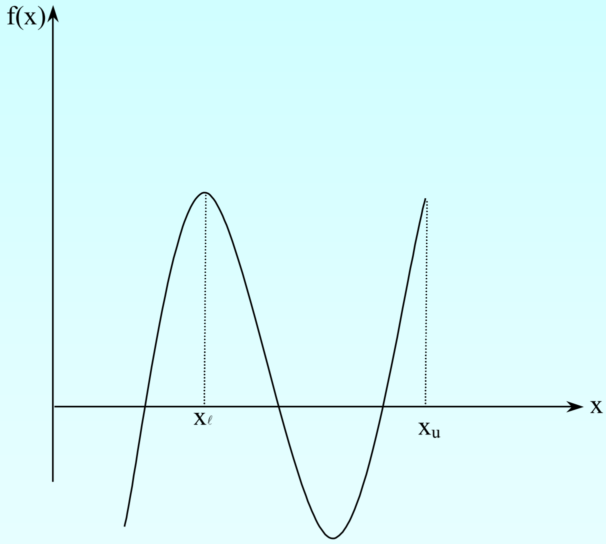
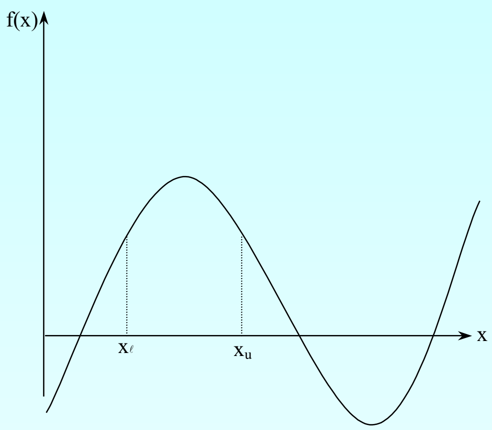


Figure 2 If function $f(x)$ does not change sign between two points, roots of the equation $f(x)=0$ may still exist between the two points.

Basis of Bisection Method



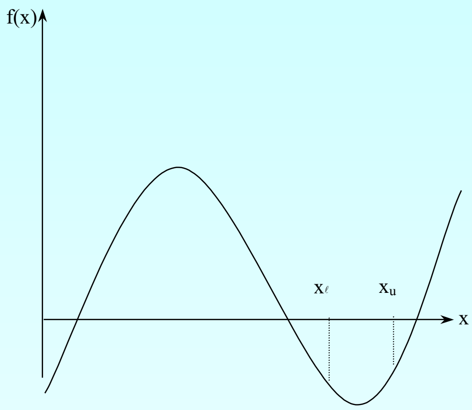


Figure 3 If the function $f(x)$ does not change sign between two points, there may not be any roots for the equation $f(x)=0$ between the two points.

Basis of Bisection Method

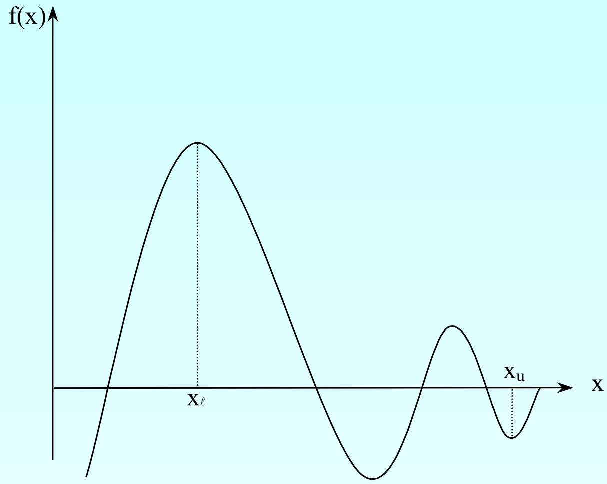


Figure 4 If the function $f(x)$ changes sign between two points, more than one root for the equation $f(x)=0$ may exist between the two points.

Algorithm for Bisection Method

Step 1

Choose x_ℓ and x_u as two guesses for the root such that $f(x_\ell)\, f(x_u) < 0$, or in other words, f(x) changes sign between x_ℓ and x_u. This was demonstrated in Figure 1.

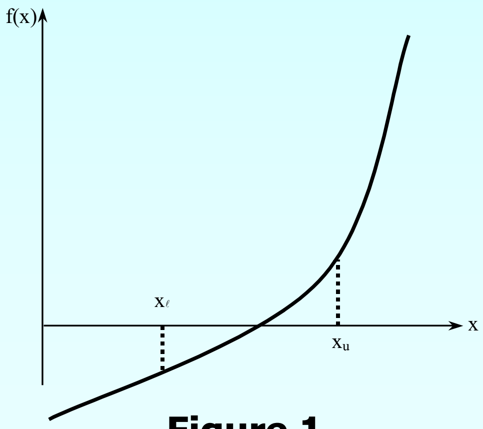


Figure 1

Step 2

Estimate the root, x_m of the equation f (x) = 0 as the mid point between x_ℓ and x_u as

$$x_m = \frac{x_\ell + x_u}{2}$$

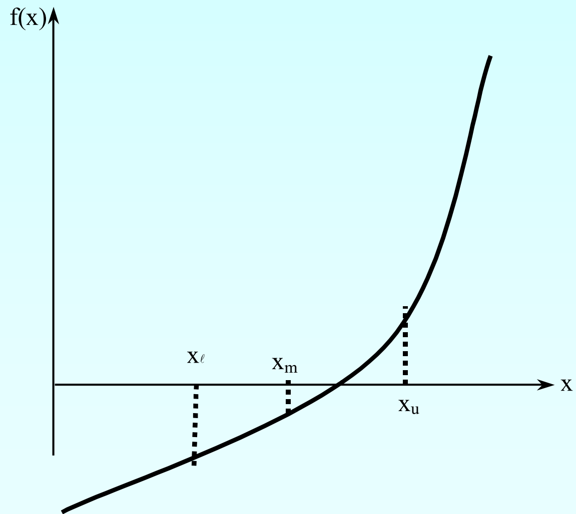


Figure 5 Estimate of x_m

Step 3

Now check the following

a) If $f(x_l)f(x_m) < 0$, then the root lies between x_ℓ and x_m; then $x_\ell = x_\ell$; $x_u = x_m$.

b) If $f(x_l)f(x_m) > 0$, then the root lies between x_m and x_u; then $x_\ell = x_m$; $x_u = x_u$.

c) If $f(x_l)f(x_m) = 0$; then the root is x_m. Stop the algorithm if this is true.

Step 4

Find the new estimate of the root

$$x_m = \frac{x_\ell + x_u}{2}$$

Find the absolute relative approximate error

$$|\in_a| = \left| \frac{x_m^{new} - x_m^{old}}{x_m^{new}} \right| \times 100$$

where

$$x_m^{old} = \text{previous estimate of root}$$

$$x_m^{new} = \text{current estimate of root}$$

Step 5

Compare the absolute relative approximate error $|\in_a|$ with the pre-specified error tolerance $\in_s$.

Is $|\in_a| > \in_s$?

Yes → Go to Step 2 using new upper and lower guesses.

No → Stop the algorithm

Note one should also check whether the number of iterations is more than the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user about it.

Example 1

You are working for 'DOWN THE TOILET COMPANY' that makes floats for ABC commodes. The floating ball has a specific gravity of 0.6 and has a radius of 5.5 cm. You are asked to find the depth to which the ball is submerged when floating in water.

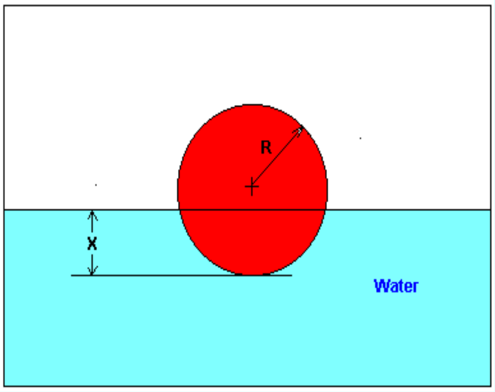


Figure 6 Diagram of the floating ball

Example 1 Cont.

The equation that gives the depth x to which the ball is submerged under water is given by

$$x^3 - 0.165x^2 + 3.993 \times 10^{-4} = 0$$

a) Use the bisection method of finding roots of equations to find the depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation.

b) Find the absolute relative approximate error at the end of each iteration, and the number of significant digits at least correct at the end of each iteration.

Example 1 Cont.

From the physics of the problem, the ball would be submerged between $x = 0$ and $x = 2R$,

where R = radius of the ball,

that is

$$0 \le x \le 2R$$
$$0 \le x \le 2(0.055)$$
$$0 \le x \le 0.11$$

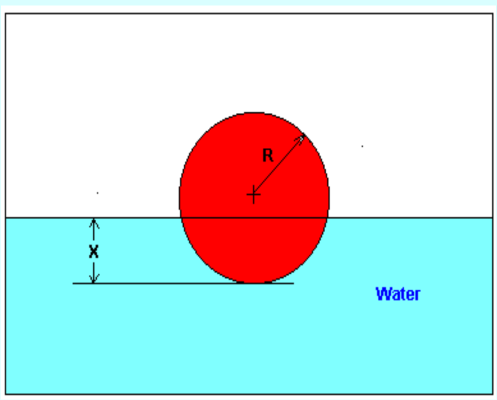


Figure 6 Diagram of the floating ball

Example 1 Cont.

Solution

To aid in the understanding of how this method works to find the root of an equation, the graph of f(x) is shown to the right,

where

$$f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4}$$

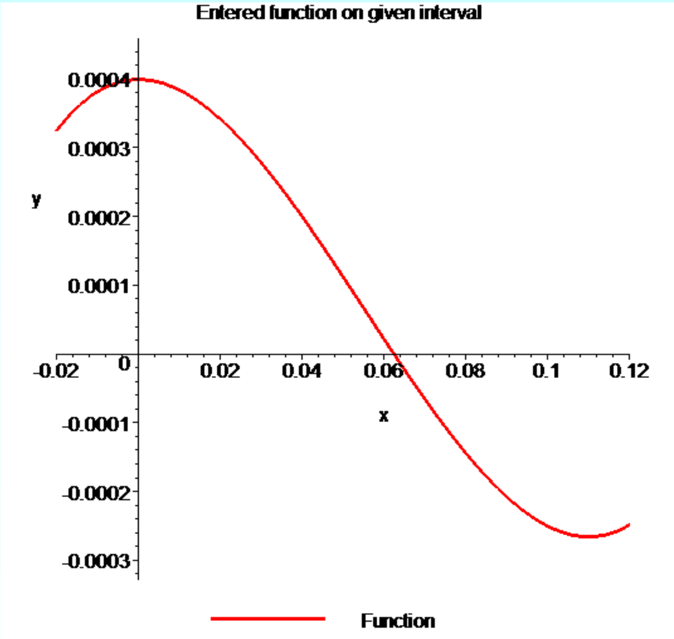


Figure 7 Graph of the function f(x)

Example 1 Cont.

Let us assume

$$x_\ell = 0.00$$

$$x_u = 0.11$$

Check if the function changes sign between x_ℓ and x_u .

$$f(x_l) = f(0) = (0)^3 - 0.165(0)^2 + 3.993 \times 10^{-4} = 3.993 \times 10^{-4}$$

$$f(x_u) = f(0.11) = (0.11)^3 - 0.165(0.11)^2 + 3.993 \times 10^{-4} = -2.662 \times 10^{-4}$$

Hence

$$f(x_l)f(x_u) = f(0)f(0.11) = (3.993 \times 10^{-4})(-2.662 \times 10^{-4}) < 0$$

So there is at least on root between x_ℓ and x_u, that is between 0 and 0.11

Example 1 Cont.

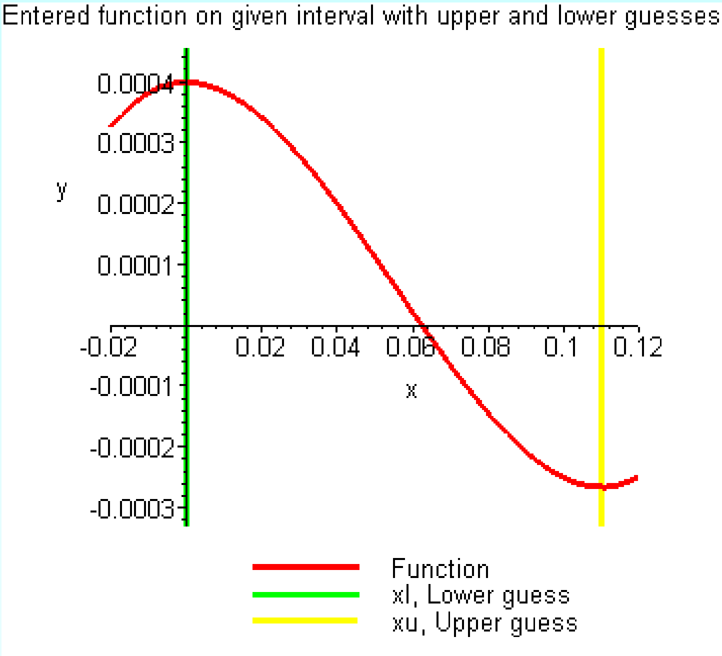


Figure 8 Graph demonstrating sign change between initial limits

Example 1 Cont.

<u>Iteration 1</u>

The estimate of the root is $x_m = \dfrac{x_\ell + x_u}{2} = \dfrac{0+0.11}{2} = 0.055$

$$f(x_m) = f(0.055) = (0.055)^3 - 0.165(0.055)^2 + 3.993\times10^{-4} = 6.655\times10^{-5}$$

$$f(x_l)f(x_m) = f(0)f(0.055) = \left(3.993\times10^{-4}\right)\left(6.655\times10^{-5}\right) > 0$$

Hence the root is bracketed between x_m and x_u, that is, between 0.055 and 0.11. So, the lower and upper limits of the new bracket are

$$x_l = 0.055,\ x_u = 0.11$$

At this point, the absolute relative approximate error $|\in_a|$ cannot be calculated as we do not have a previous approximation.

Example 1 Cont.

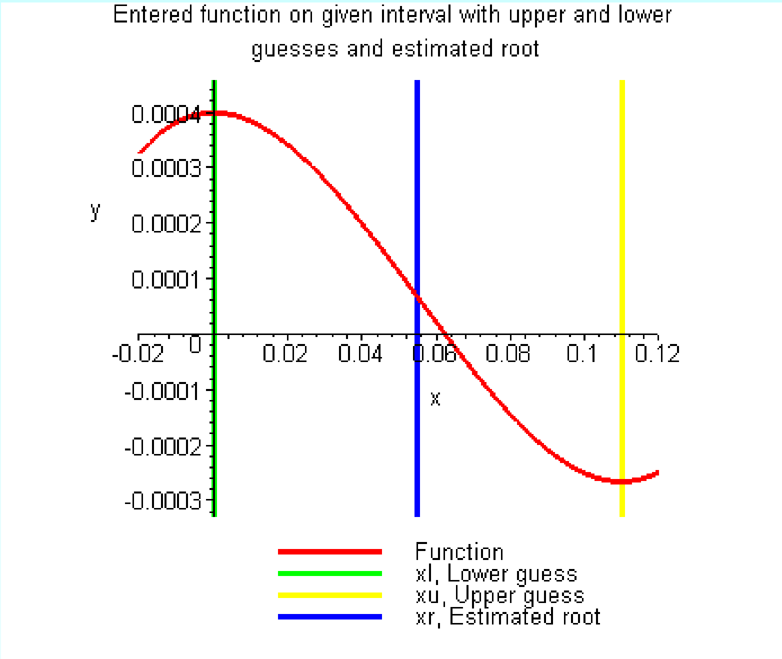


Figure 9 Estimate of the root for Iteration 1

Example 1 Cont.

<u>Iteration 2</u>

The estimate of the root is $x_m = \dfrac{x_\ell + x_u}{2} = \dfrac{0.055 + 0.11}{2} = 0.0825$

$$f(x_m) = f(0.0825) = (0.0825)^3 - 0.165(0.0825)^2 + 3.993 \times 10^{-4} = -1.622 \times 10^{-4}$$

$$f(x_l)f(x_m) = f(0.055)f(0.0825) = \left(-1.622 \times 10^{-4}\right)\left(6.655 \times 10^{-5}\right) < 0$$

Hence the root is bracketed between x_ℓ and x_m, that is, between 0.055 and 0.0825. So, the lower and upper limits of the new bracket are

$$x_l = 0.055, \; x_u = 0.0825$$

Example 1 Cont.

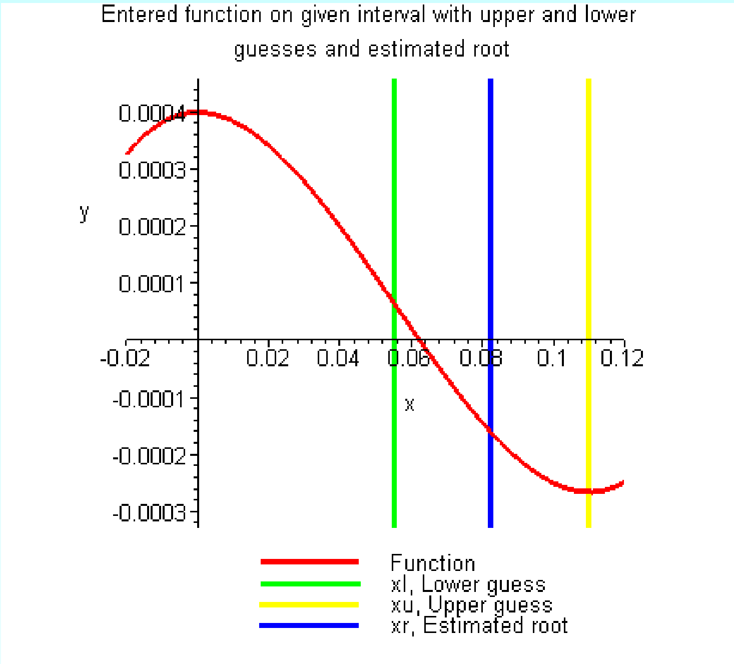


Figure 10 Estimate of the root for Iteration 2

Example 1 Cont.

The absolute relative approximate error $\left|\in_a\right|$ at the end of Iteration 2 is

$$\left|\in_a\right| = \left|\frac{x_m^{new} - x_m^{old}}{x_m^{new}}\right| \times 100$$

$$= \left|\frac{0.0825 - 0.055}{0.0825}\right| \times 100$$

$$= 33.333\%$$

None of the significant digits are at least correct in the estimate root of x_m = 0.0825 because the absolute relative approximate error is greater than 5%.

Example 1 Cont.

Iteration 3

The estimate of the root is $x_m = \dfrac{x_\ell + x_u}{2} = \dfrac{0.055 + 0.0825}{2} = 0.06875$

$$f(x_m) = f(0.06875) = (0.06875)^3 - 0.165(0.06875)^2 + 3.993\times10^{-4} = -5.563\times10^{-5}$$

$$f(x_l)f(x_m) = f(0.055)f(0.06875) = (6.655\times10^{-5})(-5.563\times10^{-5}) < 0$$

Hence the root is bracketed between x_ℓ and x_m, that is, between 0.055 and 0.06875. So, the lower and upper limits of the new bracket are

$$x_l = 0.055,\ x_u = 0.06875$$

Example 1 Cont.

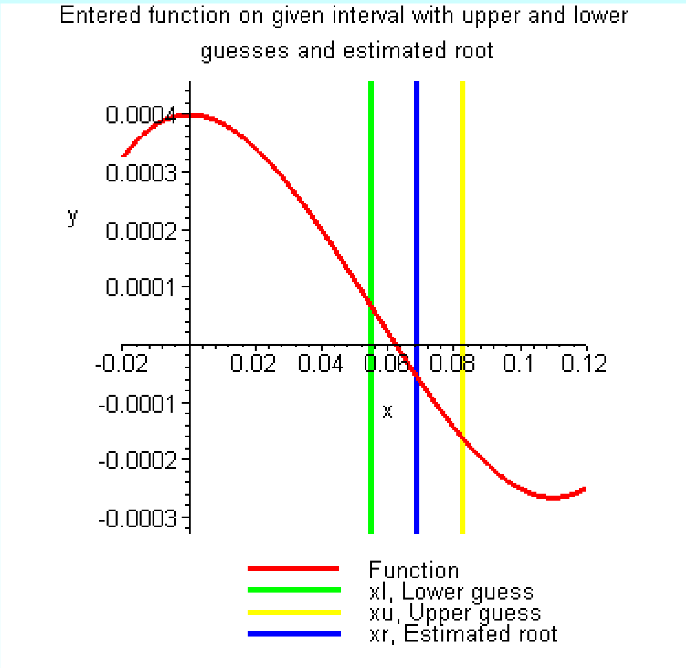


Figure 11 Estimate of the root for Iteration 3

Example 1 Cont.

The absolute relative approximate error $|\in_a|$ at the end of Iteration 3 is

$$|\in_a| = \left|\frac{x_m^{new} - x_m^{old}}{x_m^{new}}\right| \times 100$$

$$= \left|\frac{0.06875 - 0.0825}{0.06875}\right| \times 100$$

$$= 20\%$$

Still none of the significant digits are at least correct in the estimated root of the equation as the absolute relative approximate error is greater than 5%.
Seven more iterations were conducted and these iterations are shown in Table 1.

Table 1 Cont.

Table 1 Root of f(x)=0 as function of number of iterations for bisection method.

Iteration	x_ℓ	x_u	x_m	$\lvert\in_a\rvert$ %	$f(x_m)$
1	0.00000	0.11	0.055	----------	6.655×10^{-5}
2	0.055	0.11	0.0825	33.33	-1.622×10^{-4}
3	0.055	0.0825	0.06875	20.00	-5.563×10^{-5}
4	0.055	0.06875	0.06188	11.11	4.484×10^{-6}
5	0.06188	0.06875	0.06531	5.263	-2.593×10^{-5}
6	0.06188	0.06531	0.06359	2.702	-1.0804×10^{-5}
7	0.06188	0.06359	0.06273	1.370	-3.176×10^{-6}
8	0.06188	0.06273	0.0623	0.6897	6.497×10^{-7}
9	0.0623	0.06273	0.06252	0.3436	-1.265×10^{-6}
10	0.0623	0.06252	0.06241	0.1721	-3.0768×10^{-7}

Table 1 Cont.

Hence the number of significant digits at least correct is given by the largest value of *m* for which

$$|\in_a| \le 0.5 \times 10^{2-m}$$

$$0.1721 \le 0.5 \times 10^{2-m}$$

$$0.3442 \le 10^{2-m}$$

$$\log(0.3442) \le 2 - m$$

$$m \le 2 - \log(0.3442) = 2.463$$

So

$$m = 2$$

The number of significant digits at least correct in the estimated root of 0.06241 at the end of the 10th iteration is 2.

Advantages

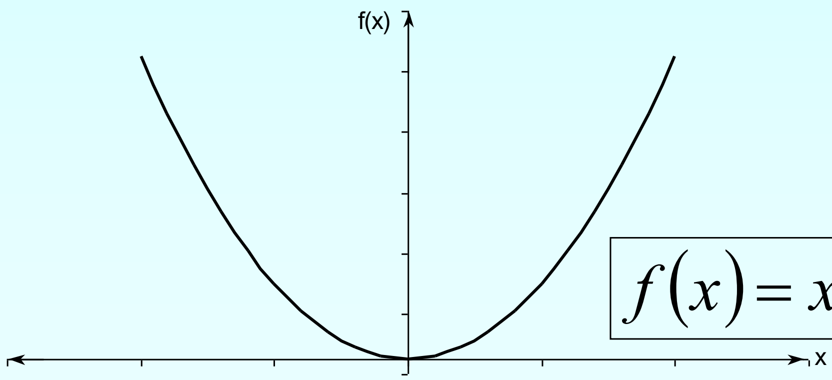
- Always convergent
- The root bracket gets halved with each iteration - guaranteed.

Drawbacks

- Slow convergence
- If one of the initial guesses is close to the root, the convergence is slower

Drawbacks (continued)

- If a function f(x) is such that it just touches the x-axis it will be unable to find the lower and upper guesses.

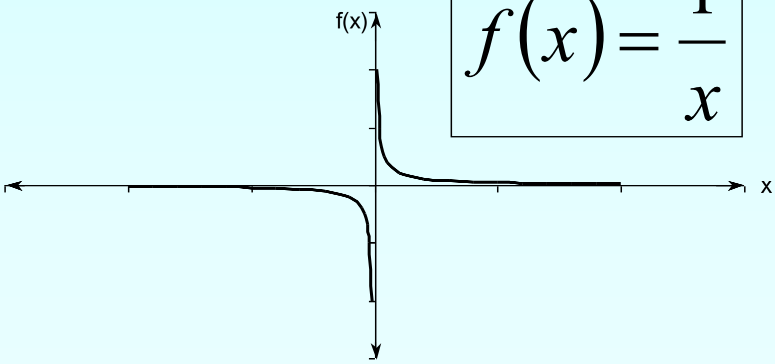


$$f(x) = x^2$$

Drawbacks (continued)

- Function changes sign but root does not exist

$$f(x) = \frac{1}{x}$$



THE END

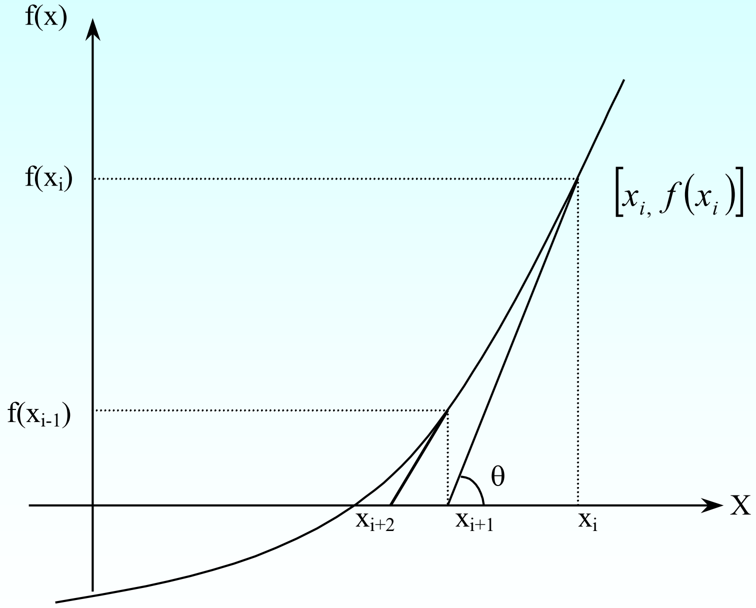
Newton-Raphson Method

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Newton-Raphson Method

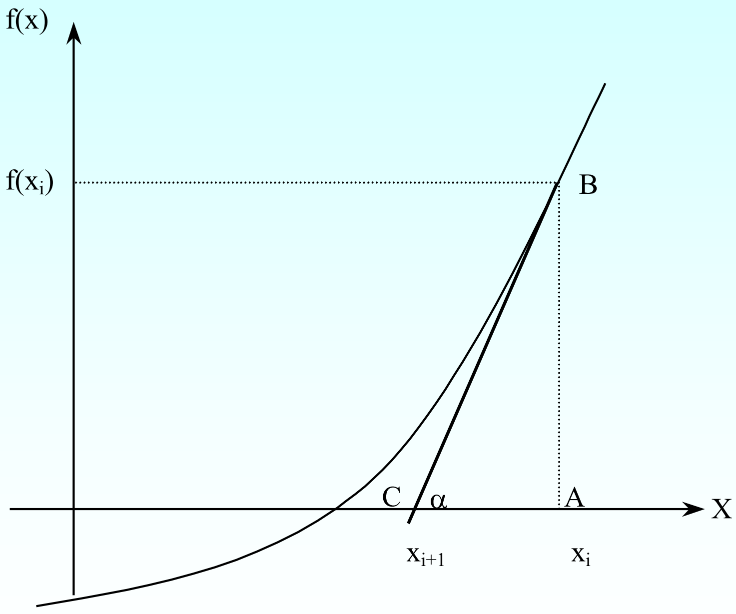
Newton-Raphson Method



$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Figure 1 Geometrical illustration of the Newton-Raphson method.

Derivation



$$\tan(\alpha) = \frac{AB}{AC}$$

$$f'(x_i) = \frac{f(x_i)}{x_i - x_{i+1}}$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Figure 2 Derivation of the Newton-Raphson method.

Algorithm for Newton-Raphson Method

Step 1

Evaluate $f'(x)$ symbolically.

Step 2

Use an initial guess of the root, x_i , to estimate the new value of the root, x_{i+1} , as

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Step 3

Find the absolute relative approximate error $|\in_a|$ as

$$|\in_a| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

Step 4

Compare the absolute relative approximate error with the pre-specified relative error tolerance $\in_s$.

Is $|\in_a| > \in_s$?

Yes → Go to Step 2 using new estimate of the root.

No → Stop the algorithm

Also, check if the number of iterations has exceeded the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user.

Example 1

You are working for 'DOWN THE TOILET COMPANY' that makes floats for ABC commodes. The floating ball has a specific gravity of 0.6 and has a radius of 5.5 cm. You are asked to find the depth to which the ball is submerged when floating in water.

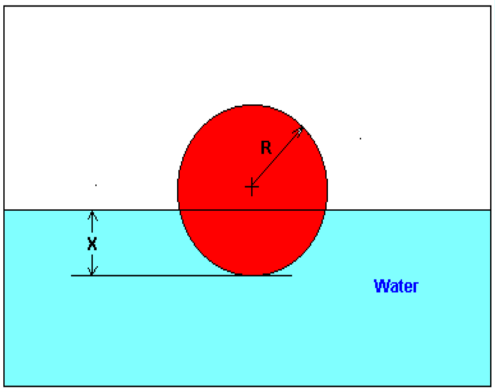


Figure 3 Floating ball problem.

Example 1 Cont.

The equation that gives the depth x in meters to which the ball is submerged under water is given by

$$f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4}$$

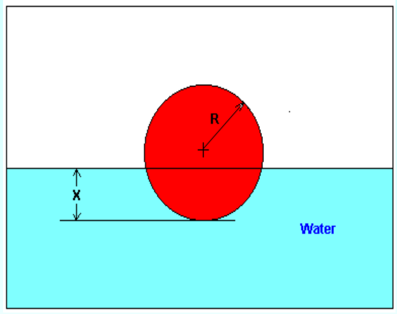


Figure 3 Floating ball problem.

Use the Newton's method of finding roots of equations to find

a) the depth 'x' to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation.
b) The absolute relative approximate error at the end of each iteration, and
c) The number of significant digits at least correct at the end of each iteration.

Example 1 Cont.

Solution

To aid in the understanding of how this method works to find the root of an equation, the graph of f(x) is shown to the right,

where

$$f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4}$$

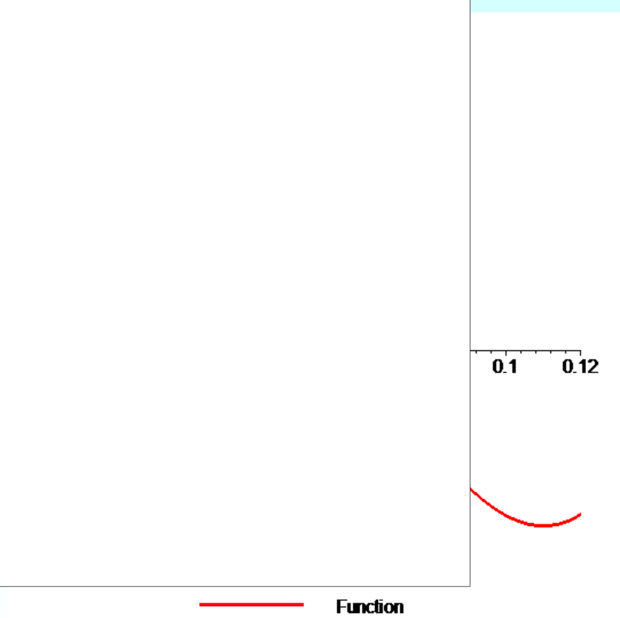


Figure 4 Graph of the function f(x)

Example 1 Cont.

Solve for $f'(x)$

$$f(x) = x^3 - 0.165x^2 + 3.993\times10^{-4}$$

$$f'(x) = 3x^2 - 0.33x$$

Let us assume the initial guess of the root of $f(x) = 0$ is $x_0 = 0.05\text{m}$. This is a reasonable guess (think why $x = 0$ and $x = 0.11\text{m}$ are not good choices) as the extreme values of the depth x would be 0 and the diameter (0.11 m) of the ball.

Example 1 Cont.

<u>Iteration 1</u>
The estimate of the root is

$$\begin{aligned} x_1 &= x_0 - \frac{f(x_0)}{f'(x_0)} \\ &= 0.05 - \frac{(0.05)^3 - 0.165(0.05)^2 + 3.993\times10^{-4}}{3(0.05)^2 - 0.33(0.05)} \\ &= 0.05 - \frac{1.118\times10^{-4}}{-9\times10^{-3}} \\ &= 0.05 - (-0.01242) \\ &= 0.06242 \end{aligned}$$

Example 1 Cont.

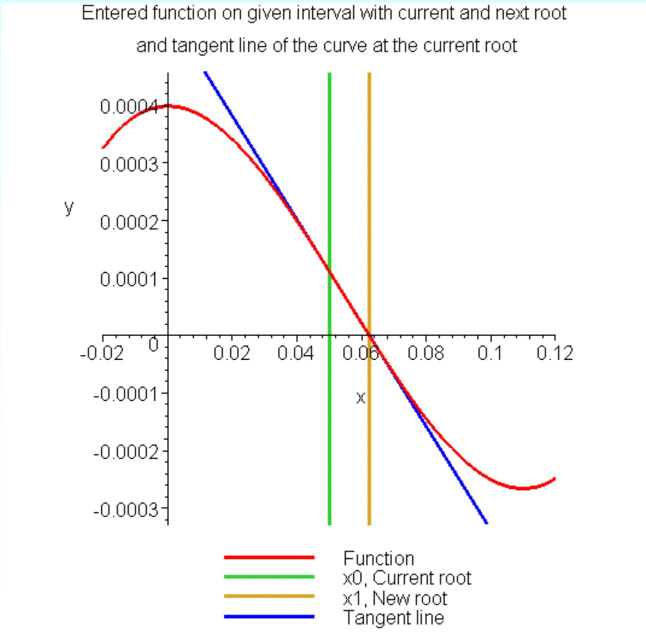


Figure 5 Estimate of the root for the first iteration.

Example 1 Cont.

The absolute relative approximate error $|\in_a|$ at the end of Iteration 1 is

$$|\in_a| = \left|\frac{x_1 - x_0}{x_1}\right| \times 100$$

$$= \left|\frac{0.06242 - 0.05}{0.06242}\right| \times 100$$

$$= 19.90\%$$

The number of significant digits at least correct is 0, as you need an absolute relative approximate error of 5% or less for at least one significant digits to be correct in your result.

Example 1 Cont.

<u>Iteration 2</u>
The estimate of the root is

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$= 0.06242 - \frac{(0.06242)^3 - 0.165(0.06242)^2 + 3.993\times10^{-4}}{3(0.06242)^2 - 0.33(0.06242)}$$

$$= 0.06242 - \frac{-3.97781\times10^{-7}}{-8.90973\times10^{-3}}$$

$$= 0.06242 - \left(4.4646\times10^{-5}\right)$$

$$= 0.06238$$

Example 1 Cont.

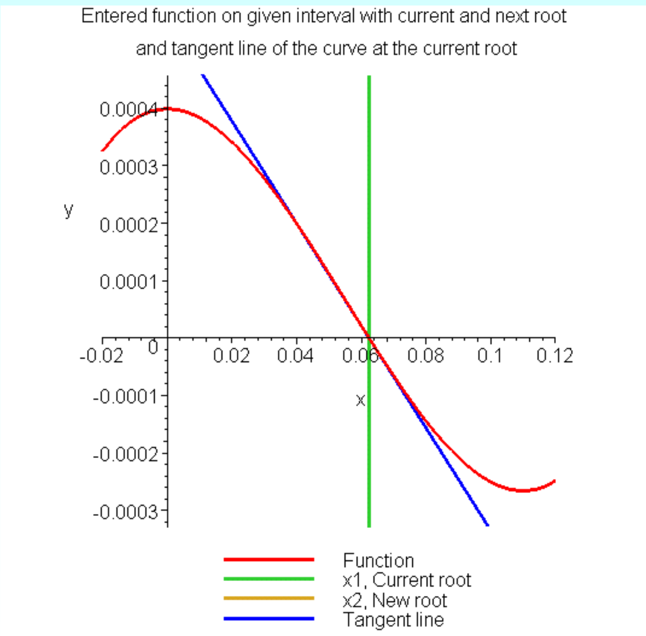


Figure 6 Estimate of the root for the Iteration 2.

Example 1 Cont.

The absolute relative approximate error $\left|\in_a\right|$ at the end of Iteration 2 is

$$\left|\in_a\right| = \left|\frac{x_2 - x_1}{x_2}\right| \times 100$$

$$= \left|\frac{0.06238 - 0.06242}{0.06238}\right| \times 100$$

$$= 0.0716\%$$

The maximum value of m for which $\left|\in_a\right| \leq 0.5 \times 10^{2-m}$ is 2.844. Hence, the number of significant digits at least correct in the answer is 2.

Example 1 Cont.

Iteration 3

The estimate of the root is

$$x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}$$

$$= 0.06238 - \frac{(0.06238)^3 - 0.165(0.06238)^2 + 3.993 \times 10^{-4}}{3(0.06238)^2 - 0.33(0.06238)}$$

$$= 0.06238 - \frac{4.44 \times 10^{-11}}{-8.91171 \times 10^{-3}}$$

$$= 0.06238 - \left(-4.9822 \times 10^{-9}\right)$$

$$= 0.06238$$

Example 1 Cont.

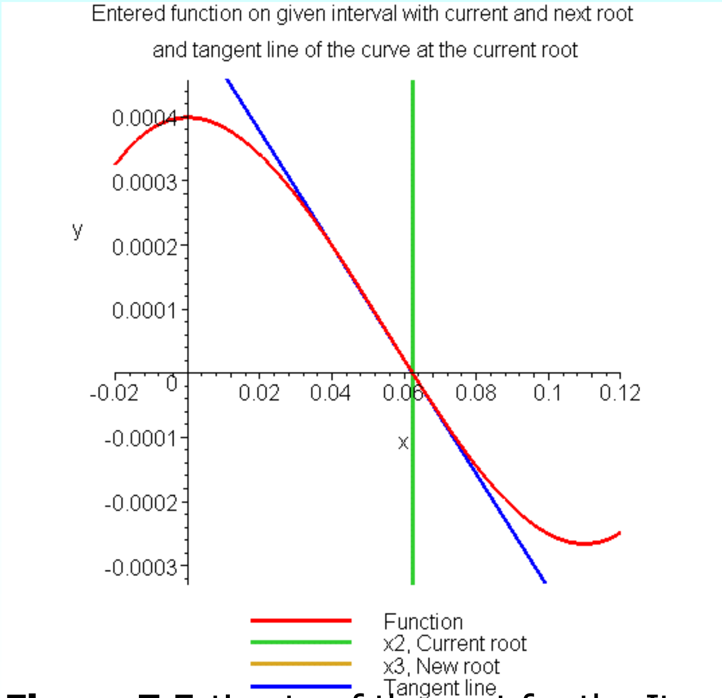


Figure 7 Estimate of the root for the Iteration 3.

Example 1 Cont.

The absolute relative approximate error $|\in_a|$ at the end of Iteration 3 is

$$|\in_a| = \left|\frac{x_2 - x_1}{x_2}\right| \times 100$$

$$= \left|\frac{0.06238 - 0.06238}{0.06238}\right| \times 100$$

$$= 0\%$$

The number of significant digits at least correct is 4, as only 4 significant digits are carried through all the calculations.

Advantages and Drawbacks of Newton Raphson Method

Advantages

- Converges fast (quadratic convergence), if it converges.
- Requires only one guess

Drawbacks

1. <u>Divergence at inflection points</u>
   Selection of the initial guess or an iteration value of the root that is close to the inflection point of the function $f(x)$ may start diverging away from the root in the Newton-Raphson method.

For example, to find the root of the equation $f(x) = (x-1)^3 + 0.512 = 0$.

The Newton-Raphson method reduces to $x_{i+1} = x_i - \dfrac{(x_i^3 - 1)^3 + 0.512}{3(x_i - 1)^2}$.

Table 1 shows the iterated values of the root of the equation.

The root starts to diverge at Iteration 6 because the previous estimate of 0.92589 is close to the inflection point of $x = 1$.

Eventually after 12 more iterations the root converges to the exact value of $x = 0.2$.

Drawbacks – Inflection Points

Table 1 Divergence near inflection point.

Iteration Number	x_i
0	5.0000
1	3.6560
2	2.7465
3	2.1084
4	1.6000
5	0.92589
6	−30.119
7	−19.746
18	0.2000

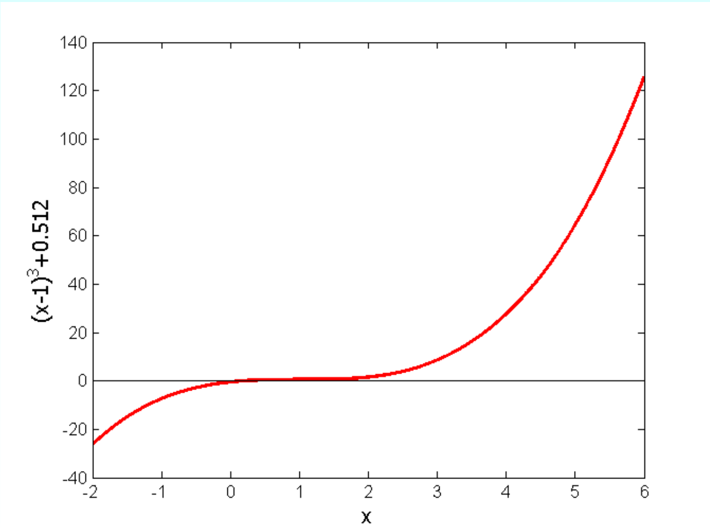


Figure 8 Divergence at inflection point for $f(x) = (x-1)^3 + 0.512 = 0$

Drawbacks – Division by Zero

2. <u>Division by zero</u>
   For the equation

$$f(x) = x^3 - 0.03x^2 + 2.4\times10^{-6} = 0$$

the Newton-Raphson method reduces to

$$x_{i+1} = x_i - \frac{x_i^3 - 0.03x_i^2 + 2.4\times10^{-6}}{3x_i^2 - 0.06x_i}$$

For $x_0 = 0$ or $x_0 = 0.02$, the denominator will equal zero.

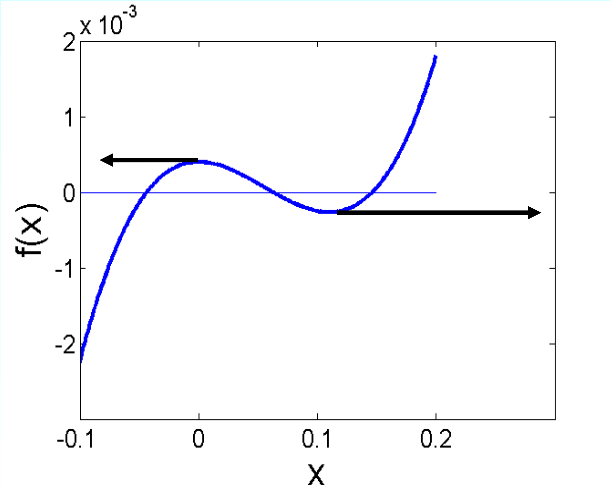


Figure 9 Pitfall of division by zero or near a zero number

Drawbacks – Oscillations near local maximum and minimum

3. <u>Oscillations near local maximum and minimum</u>

Results obtained from the Newton-Raphson method may oscillate about the local maximum or minimum without converging on a root but converging on the local maximum or minimum.

Eventually, it may lead to division by a number close to zero and may diverge.

For example for $f(x) = x^2 + 2 = 0$ the equation has no real roots.

Drawbacks – Oscillations near local maximum and minimum

Table 3 Oscillations near local maxima and mimima in Newton-Raphson method.

Iteration Number	x_i	$f(x_i)$	$\lvert\in_a\rvert\%$
0	–1.0000	3.00	
1	0.5	2.25	300.00
2	–1.75	5.063	128.571
3	–0.30357	2.092	476.47
4	3.1423	11.874	109.66
5	1.2529	3.570	150.80
6	–0.17166	2.029	829.88
7	5.7395	34.942	102.99
8	2.6955	9.266	112.93
9	0.97678	2.954	175.96

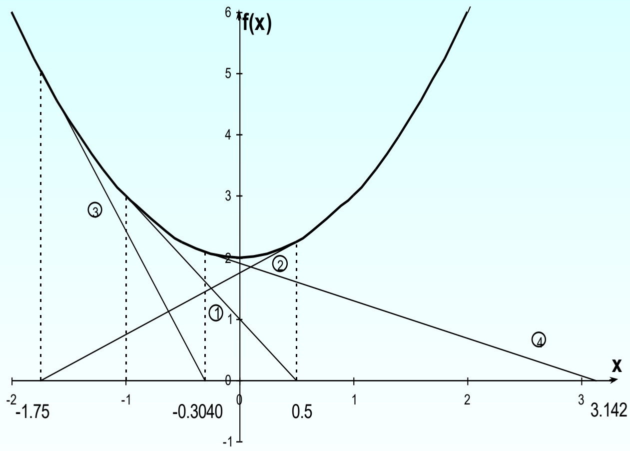


Figure 10 Oscillations around local minima for $f(x) = x^2 + 2$.

Drawbacks – Root Jumping

4. Root Jumping

In some cases where the function $f(x)$ is oscillating and has a number of roots, one may choose an initial guess close to a root. However, the guesses may jump and converge to some other root.

For example

$$f(x) = \sin x = 0$$

Choose

$$x_0 = 2.4\pi = 7.539822$$

It will converge to $x = 0$

instead of $x = 2\pi = 6.2831853$

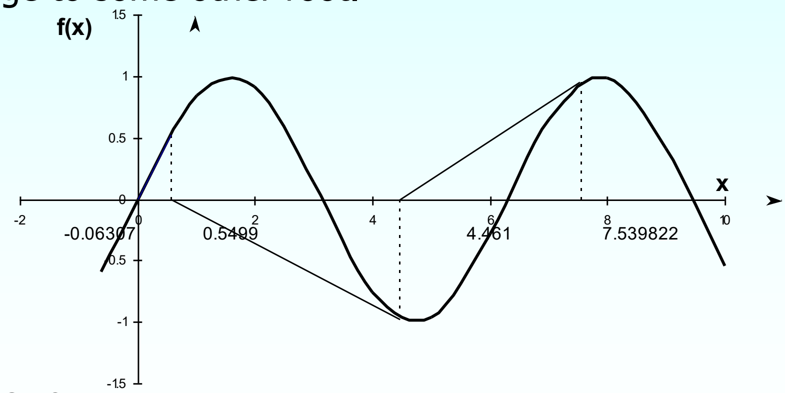


Figure 11 Root jumping from intended location of root for $f(x) = \sin x = 0$

THE END

Gaussian Elimination

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Naïve Gauss Elimination

System of Linear Equations

A system of n linear equations: a set of *n* equations and *n* unknowns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2$$

$$\vdots \qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = b_n$$

System of Linear Equations

A system of n linear equations: Matrix Form

A linear system might be described by the following equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

These equations could be written in matrix form as:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

The matrix equation could be written as: $\mathbf{Ax = b}$

Naïve Gaussian Elimination

A method to solve simultaneous linear equations of the form [A][X]=[C]

Two steps

1. Forward Elimination
2. Back Substitution

Forward Elimination

The goal of forward elimination is to transform the coefficient matrix into an upper triangular matrix

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Forward Elimination

A set of *n* equations and *n* unknowns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2$$

$$\vdots \qquad\qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = b_n$$

(n-1) steps of forward elimination

Forward Elimination

Step 1

For Equation 2, divide Equation 1 by a_{11} and multiply by a_{21}.

$$\left[\frac{a_{21}}{a_{11}}\right](a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1)$$

$$a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \ldots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1$$

Forward Elimination

Subtract the result from Equation 2.

$$\begin{array}{rl} & a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2 \\ - & a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \ldots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1 \\ \hline & \left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \ldots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)x_n = b_2 - \frac{a_{21}}{a_{11}}b_1 \end{array}$$

or $\quad a'_{22}x_2 + \ldots + a'_{2n}x_n = b'_2$

Forward Elimination

Repeat this procedure for the remaining equations to reduce the set of equations as

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a'_{32}x_2 + a'_{33}x_3 + \ldots + a'_{3n}x_n &= b'_3 \\
\vdots \qquad \vdots \qquad \qquad \vdots \\
a'_{n2}x_2 + a'_{n3}x_3 + \ldots + a'_{nn}x_n &= b'_n
\end{aligned}
$$

End of Step 1

Forward Elimination

Step 2

Repeat the same procedure for the 3rd term of Equation 3.

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{3n}x_n &= b''_3 \\
\vdots \qquad \vdots \\
a''_{n3}x_3 + \ldots + a''_{nn}x_n &= b''_n
\end{aligned}
$$

End of Step 2

Forward Elimination

At the end of (n-1) Forward Elimination steps, the system of equations will look like

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a_{22}'x_2 + a_{23}'x_3 + \ldots + a_{2n}'x_n &= b_2' \\
a_{33}''x_3 + \ldots + a_{3n}''x_n &= b_3'' \\
\vdots \quad & \quad \vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1)}
\end{aligned}
$$

End of Step (n-1)

Matrix Form at End of Forward Elimination

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
0 & a_{22}' & a_{23}' & \cdots & a_{2n}' \\
0 & 0 & a_{33}'' & \cdots & a_{3n}'' \\
\vdots & \vdots & \vdots & \cdots & \vdots \\
0 & 0 & 0 & 0 & a_{nn}^{(n-1)}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}
=
\begin{bmatrix} b_1 \\ b_2' \\ b_3'' \\ \vdots \\ b_n^{(n-1)} \end{bmatrix}
$$

Back Substitution

Solve each equation starting from the last equation

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Example of a system of 3 equations

Back Substitution Starting Eqns

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\ a''_{33}x_3 + \ldots + a''_{n}x_n &= b''_3 \\ \vdots \qquad & \ \ \vdots \\ a_{nn}^{(n-1)}x_n &= b_n^{(n-1\ )} \end{aligned}$$

Back Substitution

Start with the last equation because it has only one unknown

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

Back Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - a_{i,i+1}^{(i-1)} x_{i+1} - a_{i,i+2}^{(i-1)} x_{i+2} - \ldots - a_{i,n}^{(i-1)} x_n}{a_{ii}^{(i-1)}} \text{ for } i = n-1, \ldots, 1$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}} \text{ for } i = n-1, \ldots, 1$$

Naïve Gauss Elimination Example

Example 1

The upward velocity of a rocket is given at three different times

Table 1 Velocity vs. time data.

Time, $t\ (\mathrm{s})$	**Velocity,** $v\ (\mathrm{m/s})$
5	106.8
8	177.2
12	279.2

The velocity data is approximated by a polynomial as:

$$v(t) = a_1 t^2 + a_2 t + a_3 \ , \qquad 5 \le \mathrm{t} \le 12.$$

Find the velocity at t=6 seconds .

Example 1 Cont.

Assume

$$v(t) = a_1 t^2 + a_2 t + a_3 \;, \quad 5 \le t \le 12.$$

Results in a matrix template of the form:

$$\begin{bmatrix} t_1^2 & t_1 & 1 \\ t_2^2 & t_2 & 1 \\ t_3^2 & t_3 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

Using data from Table 1, the matrix becomes:

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Example 1 Cont.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

1. Forward Elimination
2. Back Substitution

Forward Elimination

Number of Steps of Forward Elimination

Number of steps of forward elimination is $(n-1)=(3-1)=2$

Forward Elimination: Step 1

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Divide Equation 1 by 25 and multiply it by 64, $\frac{64}{25} = 2.56$.

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix} \times 2.56 = \begin{bmatrix} 64 & 12.8 & 2.56 & \vdots & 273.408 \end{bmatrix}$$

Subtract the result from Equation 2

$$\begin{array}{r} \begin{bmatrix} 64 & 8 & 1 & \vdots & 177.2 \end{bmatrix} \\ -\begin{bmatrix} 64 & 12.8 & 2.56 & \vdots & 273.408 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & -4.8 & -1.56 & \vdots & -96.208 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Divide Equation 1 by 25 and multiply it by 144, $\frac{144}{25} = 5.76$.

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix} \times 5.76 = \begin{bmatrix} 144 & 28.8 & 5.76 & \vdots & 615.168 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \\ -\begin{bmatrix} 144 & 28.8 & 5.76 & \vdots & 615.168 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$

Forward Elimination: Step 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$

Divide Equation 2 by −4.8 and multiply it by −16.8, $\frac{-16.8}{-4.8} = 3.5$.

$$\begin{bmatrix} 0 & -4.8 & -1.56 & \vdots & -96.208 \end{bmatrix} \times 3.5 = \begin{bmatrix} 0 & -16.8 & -5.46 & \vdots & -336.728 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 0 & -16.8 & -4.76 & \vdots & 335.968 \end{bmatrix} \\ -\begin{bmatrix} 0 & -16.8 & -5.46 & \vdots & -336.728 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 0 & 0.7 & \vdots & 0.76 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & 0 & 0.7 & \vdots & 0.76 \end{bmatrix}$$

Back Substitution

Back Substitution

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.2 \\ 0 & 0 & 0.7 & \vdots & 0.7 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for a_3

$$0.7a_3 = 0.76$$

$$a_3 = \frac{0.76}{0.7}$$

$$a_3 = 1.08571$$

Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for a_2

$$-4.8a_2 - 1.56a_3 = -96.208$$

$$a_2 = \frac{-96.208 + 1.56a_3}{-4.8}$$

$$a_2 = \frac{-96.208 + 1.56 \times 1.08571}{-4.8}$$

$$a_2 = 19.6905$$

Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.2 \\ 0.76 \end{bmatrix}$$

Solving for a_1

$$25a_1 + 5a_2 + a_3 = 106.8$$

$$\begin{aligned} a_1 &= \frac{106.8 - 5a_2 - a_3}{25} \\ &= \frac{106.8 - 5 \times 19.6905 - 1.08571}{25} \\ &= 0.290472 \end{aligned}$$

Naïve Gaussian Elimination Solution

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

Example 1 Cont.

Solution

The solution vector is

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

The polynomial that passes through the three data points is then:

$$\begin{aligned} v(t) &= a_1 t^2 + a_2 t + a_3 \\ &= 0.290472t^2 + 19.6905t + 1.08571, \quad 5 \le t \le 12 \end{aligned}$$

$$\begin{aligned} v(6) &= 0.290472(6)^2 + 19.6905(6) + 1.08571 \\ &= 129.686 \text{ m/s.} \end{aligned}$$

THE END

Naïve Gauss Elimination Partial Pivoting

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Naïve Gauss Elimination Pitfalls

Pitfall#1. Division by zero

$$10x_2 - 7x_3 = 3$$
$$6x_1 + 2x_2 + 3x_3 = 11$$
$$5x_1 - x_2 + 5x_3 = 9$$

$$\begin{bmatrix} 0 & 10 & -7 \\ 6 & 2 & 3 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 11 \\ 9 \end{bmatrix}$$

Is division by zero an issue here?

$$12x_1 + 10x_2 - 7x_3 = 15$$
$$6x_1 + 5x_2 + 3x_3 = 14$$
$$5x_1 - x_2 + 5x_3 = 9$$

$$\begin{bmatrix} 12 & 10 & -7 \\ 6 & 5 & 3 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 14 \\ 9 \end{bmatrix}$$

Is division by zero an issue here? YES

$$12x_1 + 10x_2 - 7x_3 = 15$$
$$6x_1 + 5x_2 + 3x_3 = 14$$
$$24x_1 - x_2 + 5x_3 = 28$$

$$\begin{bmatrix} 12 & 10 & -7 \\ 6 & 5 & 3 \\ 24 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 14 \\ 28 \end{bmatrix} \longrightarrow \begin{bmatrix} 12 & 10 & -7 \\ 0 & 0 & 6.5 \\ 12 & -21 & 19 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15 \\ 6.5 \\ -2 \end{bmatrix}$$

Division by zero is a possibility at any step of forward elimination

Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Exact Solution

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Solve it on a computer using 6 significant digits with chopping

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.9625 \\ 1.05 \\ 0.999995 \end{bmatrix}$$

Pitfall#2. Large Round-off Errors

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Solve it on a computer using 5 significant digits with chopping

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.625 \\ 1.5 \\ 0.99995 \end{bmatrix}$$

Is there a way to reduce the round off error?

Avoiding Pitfalls

Increase the number of significant digits

- Decreases round-off error
- Does not avoid division by zero

Avoiding Pitfalls

Gaussian Elimination with Partial Pivoting

- Avoids division by zero
- Reduces round off error

Gauss Elimination with Partial Pivoting

Pitfalls of Naïve Gauss Elimination

- Possible division by zero
- Large round-off errors

Avoiding Pitfalls

Increase the number of significant digits

- Decreases round-off error
- Does not avoid division by zero

Avoiding Pitfalls

Gaussian Elimination with Partial Pivoting

- Avoids division by zero
- Reduces round off error

What is Different About Partial Pivoting?

At the beginning of the k^{th} step of forward elimination, find the maximum of

$$|a_{kk}|, |a_{k+1,k}|, \ldots\ldots\ldots\ldots\ldots, |a_{nk}|$$

If the maximum of the values is $|a_{pk}|$

in the p^{th} row, $k \le p \le n,$ then switch rows p and k.

Matrix Form at Beginning of 2nd Step of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & a'_{n3} & a'_{n4} & a'_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b'_3 \\ \vdots \\ b'_n \end{bmatrix}$$

Example (2nd step of FE)

$$\begin{bmatrix} 6 & 14 & 5.1 & 3.7 & 6 \\ 0 & -7 & 6 & 1 & 2 \\ 0 & 4 & 12 & 1 & 11 \\ 0 & 9 & 23 & 6 & 8 \\ 0 & -17 & 12 & 11 & 43 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 5 \\ -6 \\ 8 \\ 9 \\ 3 \end{bmatrix}$$

Which two rows would you switch?

Example (2nd step of FE)

$$\begin{bmatrix} 6 & 14 & 5.1 & 3.7 & 6 \\ 0 & -17 & 12 & 11 & 43 \\ 0 & 4 & 12 & 1 & 11 \\ 0 & 9 & 23 & 6 & 8 \\ 0 & -7 & 6 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ 8 \\ 9 \\ -6 \end{bmatrix}$$

Switched Rows

Gaussian Elimination with Partial Pivoting

A method to solve simultaneous linear equations of the form [A][X]=[C]

Two steps

1. Forward Elimination
2. Back Substitution

Forward Elimination

Same as naïve Gauss elimination method except that we switch rows before **each** of the (n-1) steps of forward elimination.

Example: Matrix Form at Beginning of 2nd Step of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & a'_{32} & a'_{33} & \cdots & a'_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & a'_{n3} & a'_{n4} & a'_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b'_3 \\ \vdots \\ b'_n \end{bmatrix}$$

Matrix Form at End of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & 0 & a''_{33} & \cdots & a''_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & a_{nn}^{(n-1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \\ \vdots \\ b_n^{(n-1)} \end{bmatrix}$$

Back Substitution Starting Eqns

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{n}x_n &= b''_3 \\
\vdots \qquad & \quad \vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1)}
\end{aligned}
$$

Back Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}} \text{ for } i = n-1,\ldots,1$$

Gauss Elimination with Partial Pivoting Example

Example 2

Solve the following set of equations by Gaussian elimination with partial pivoting

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Example 2 Cont.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

1. Forward Elimination
2. Back Substitution

Forward Elimination

Number of Steps of Forward Elimination

Number of steps of forward elimination is $(n-1)=(3-1)=2$

Forward Elimination: Step 1

- Examine absolute values of first column, first row and below.

$$|25|,|64|,|144|$$

- Largest absolute value is 144 and exists in row 3.
- Switch row 1 and row 3.

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

Divide Equation 1 by 144 and multiply it by 64, $\frac{64}{144} = 0.4444$.

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \times 0.4444 = \begin{bmatrix} 63.99 & 5.333 & 0.4444 & \vdots & 124.1 \end{bmatrix}$$

Subtract the result from Equation 2

$$\begin{array}{r} \begin{bmatrix} 64 & 8 & 1 & \vdots & 177.2 \end{bmatrix} \\ -\begin{bmatrix} 63.99 & 5.333 & 0.4444 & \vdots & 124.1 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix}$$

Divide Equation 1 by 144 and multiply it by 25, $\frac{25}{144} = 0.1736$.

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix} \times 0.1736 = \begin{bmatrix} 25.00 & 2.083 & 0.1736 & \vdots & 48.47 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix} \\ -\begin{bmatrix} 25 & 2.083 & 0.1736 & \vdots & 48.47 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix}$$

Forward Elimination: Step 2

- Examine absolute values of second column, second row and below.

$$|2.667|,|2.917|$$

- Largest absolute value is 2.917 and exists in row 3.
- Switch row 2 and row 3.

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix}$$

Forward Elimination: Step 2 (cont.)

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix}$$

Divide Equation 2 by 2.917 and multiply it by 2.667,

$$\frac{2.667}{2.917} = 0.9143.$$

$$\begin{bmatrix} 0 & 2.917 & 0.8264 & \vdots & 58.33 \end{bmatrix} \times 0.9143 = \begin{bmatrix} 0 & 2.667 & 0.7556 & \vdots & 53.33 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 0 & 2.667 & 0.5556 & \vdots & 53.10 \end{bmatrix} \\ -\begin{bmatrix} 0 & 2.667 & 0.7556 & \vdots & 53.33 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix}$$

Back Substitution

Back Substitution

$$\begin{bmatrix} 144 & 12 & 1 & \vdots & 279.2 \\ 0 & 2.917 & 0.8264 & \vdots & 58.33 \\ 0 & 0 & -0.2 & \vdots & -0.23 \end{bmatrix} \Rightarrow \begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for a_3

$$-0.2a_3 = -0.23$$

$$a_3 = \frac{-0.23}{-0.2}$$

$$= 1.15$$

Back Substitution (cont.)

$$\begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for a_2

$$2.917a_2 + 0.8264a_3 = 58.33$$

$$a_2 = \frac{58.33 - 0.8264a_3}{2.917}$$

$$= \frac{58.33 - 0.8264 \times 1.15}{2.917}$$

$$= 19.67$$

Back Substitution (cont.)

$$\begin{bmatrix} 144 & 12 & 1 \\ 0 & 2.917 & 0.8264 \\ 0 & 0 & -0.2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 279.2 \\ 58.33 \\ -0.23 \end{bmatrix}$$

Solving for a_1

$$144a_1 + 12a_2 + a_3 = 279.2$$

$$a_1 = \frac{279.2 - 12a_2 - a_3}{144}$$

$$= \frac{279.2 - 12 \times 19.67 - 1.15}{144}$$

$$= 0.2917$$

Gaussian Elimination with Partial Pivoting Solution

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.2917 \\ 19.67 \\ 1.15 \end{bmatrix}$$

Gauss Elimination with Partial Pivoting Another Example

Partial Pivoting: Example

Consider the system of equations

$$10x_1 - 7x_2 = 7$$

$$-3x_1 + 2.099x_2 + 6x_3 = 3.901$$

$$5x_1 - x_2 + 5x_3 = 6$$

In matrix form

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

Solve using Gaussian Elimination with Partial Pivoting using five significant digits with chopping

Partial Pivoting: Example

Forward Elimination: Step 1

Examining the values of the first column

|10|, |-3|, and |5| or 10, 3, and 5

The largest absolute value is 10, which means, to follow the rules of Partial Pivoting, we switch row1 with row1.

Performing Forward Elimination

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix}$$

Partial Pivoting: Example

Forward Elimination: Step 2

Examining the values of the first column

|-0.001| and |2.5| or 0.0001 and 2.5

The largest absolute value is 2.5, so row 2 is switched with row 3

Performing the row swap

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.001 & 6 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.001 \end{bmatrix}$$

Partial Pivoting: Example

Forward Elimination: Step 2

Performing the Forward Elimination results in:

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

Partial Pivoting: Example

Back Substitution

Solving the equations through back substitution

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

$$x_3 = \frac{6.002}{6.002} = 1$$

$$x_2 = \frac{2.5 - 5x_3}{2.5} = -1$$

$$x_1 = \frac{7 + 7x_2 - 0x_3}{10} = 0$$

Partial Pivoting: Example

Compare the calculated and exact solution

The fact that they are equal is coincidence, but it does illustrate the advantage of Partial Pivoting

$$[X]_{calculated} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \qquad [X]_{exact} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

THE END

LU Decomposition

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

LU Decomposition

LU Decomposition is another method to solve a set of simultaneous linear equations

Which is better, Gauss Elimination or LU Decomposition?

To answer this, a closer look at LU decomposition is needed.

LU Decomposition

Method

For most non-singular matrix [*A*] that one could conduct Naïve Gauss Elimination forward elimination steps, one can always write it as

$$[A] = [L][U]$$

where

$[L]$ = lower triangular matrix

$[U]$ = upper triangular matrix

How does LU Decomposition work?

If solving a set of linear equations	$[A][X] = [C]$
If $[A] = [L][U]$ then	$[L][U][X] = [C]$
Multiply by	$[L]^{-1}$
Which gives	$[L]^{-1}[L][U][X] = [L]^{-1}[C]$
Remember $[L]^{-1}[L] = [I]$ which leads to	$[I][U][X] = [L]^{-1}[C]$
Now, if $[I][U] = [U]$ then	$[U][X] = [L]^{-1}[C]$
Now, let	$[L]^{-1}[C]=[Z]$
Which ends with	$[L][Z] = [C] \quad (1)$
and	$[U][X] = [Z] \quad (2)$

LU Decomposition

How can this be used?

Given $[A][X] = [C]$

1. Decompose $[A]$ into $[L]$ and $[U]$
2. Solve $[L][Z] = [C]$ for $[Z]$
3. Solve $[U][X] = [Z]$ for $[X]$

Is LU Decomposition better than Gaussian Elimination?

Solve $[A][X]=[B]$

T = clock cycle time and nxn = size of the matrix

Forward Elimination

$$CT|_{FE}=T\left(\frac{8n^3}{3}+8n^2-\frac{32n}{3}\right)$$

Back Substitution

$$CT|_{BS}=T\left(4n^2+12n\right)$$

Decomposition to LU

$$CT|_{DE}=T\left(\frac{8n^3}{3}+4n^2-\frac{20n}{3}\right)$$

Forward Substitution

$$CT|_{FS}=T\left(4n^2-4n\right)$$

Back Substitution

$$CT|_{BS}=T\left(4n^2+12n\right)$$

Is LU Decomposition better than Gaussian Elimination?

To solve $[A][X]=[B]$

Time taken by methods

Gaussian Elimination	LU Decomposition
$T\left(\frac{8n^3}{3}+12n^2+\frac{4n}{3}\right)$	$T\left(\frac{8n^3}{3}+12n^2+\frac{4n}{3}\right)$

T = clock cycle time and nxn = size of the matrix

So both methods are equally efficient.

To find inverse of [A]

Time taken by Gaussian Elimination

$$= n\left(CT|_{FE} + CT|_{BS}\right)$$

$$= T\left(\frac{8n^4}{3} + 12n^3 + \frac{4n^2}{3}\right)$$

Time taken by LU Decomposition

$$= CT|_{DE} + n \times CT|_{FS} + n \times CT|_{BS}$$

$$= T\left(\frac{32n^3}{3} + 12n^2 - \frac{20n}{3}\right)$$

To find inverse of [A]

Time taken by Gaussian Elimination

$$T\left(\frac{8n^4}{3} + 12n^3 + \frac{4n^2}{3}\right)$$

Time taken by LU Decomposition

$$T\left(\frac{32n^3}{3} + 12n^2 - \frac{20n}{3}\right)$$

Table 1 Comparing computational times of finding inverse of a matrix using LU decomposition and Gaussian elimination.

n	10	100	1000	10000
$CT\|_{\text{inverse GE}} / CT\|_{\text{inverse LU}}$	3.288	25.84	250.8	2501

For large n, $CT|_{\text{inverse GE}} / CT|_{\text{inverse LU}} \approx n/4$

Method: [A] Decomposes to [L] and [U]

$$[A]=[L][U]=\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

[*U*] is the same as the coefficient matrix at the end of the forward elimination step.

[*L*] is obtained using the *multipliers* that were used in the forward elimination process

Finding the [*U*] matrix

Using the Forward Elimination Procedure of Gauss Elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

Step 1: $\frac{64}{25}=2.56; \quad Row2-Row1(2.56)=\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 144 & 12 & 1 \end{bmatrix}$

$$\frac{144}{25}=5.76; \quad Row3-Row1(5.76)=\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$$

Finding the [U] Matrix

Matrix after Step 1: $\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$

Step 2: $\dfrac{-16.8}{-4.8} = 3.5; \quad Row3 - Row2(3.5) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$

$$[U] = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

Finding the [L] matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}$$

Using the multipliers used during the Forward Elimination Procedure

From the first step of forward elimination $\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$

$$\ell_{21} = \frac{a_{21}}{a_{11}} = \frac{64}{25} = 2.56$$

$$\ell_{31} = \frac{a_{31}}{a_{11}} = \frac{144}{25} = 5.76$$

Finding the [L] Matrix

From the second step of forward elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix} \qquad \ell_{32} = \frac{a_{32}}{a_{22}} = \frac{-16.8}{-4.8} = 3.5$$

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}$$

Does [L][U] = [A]?

$$[L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} = \ ?$$

Using LU Decomposition to solve SLEs

Solve the following set of linear equations using LU Decomposition

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Using the procedure for finding the [*L*] and [*U*] matrices

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

Example

Set $[L][Z] = [C]$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Solve for $[Z]$

$$z_1 = 10$$
$$2.56 z_1 + z_2 = 177.2$$
$$5.76 z_1 + 3.5 z_2 + z_3 = 279.2$$

Example

Complete the forward substitution to solve for $[Z]$

$$\begin{aligned}
z_1 &= 106.8 \\
z_2 &= 177.2 - 2.56 z_1 \\
&= 177.2 - 2.56(106.8) \\
&= -96.2 \\
z_3 &= 279.2 - 5.76 z_1 - 3.5 z_2 \\
&= 279.2 - 5.76(106.8) - 3.5(-96.21) \\
&= 0.735
\end{aligned}$$

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Example

Set $[U][X] = [Z]$

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Solve for $[X]$

The 3 equations become

$$\begin{aligned}
25a_1 + 5a_2 + a_3 &= 106.8 \\
-4.8a_2 - 1.56a_3 &= -96.21 \\
0.7a_3 &= 0.735
\end{aligned}$$

Example

From the 3rd equation

$$0.7a_3 = 0.735$$

$$a_3 = \frac{0.735}{0.7}$$

$$a_3 = 1.050$$

Substituting in a_3 and using the second equation

$$-4.8a_2 - 1.56a_3 = -96.21$$

$$a_2 = \frac{-96.21 + 1.56a_3}{-4.8}$$

$$a_2 = \frac{-96.21 + 1.56(1.050)}{-4.8}$$

$$a_2 = 19.70$$

Example

Substituting in a_3 and a_2 using the first equation

$$25a_1 + 5a_2 + a_3 = 106.8$$

$$a_1 = \frac{106.8 - 5a_2 - a_3}{25}$$

$$= \frac{106.8 - 5(19.70) - 1.050}{25}$$

$$= 0.2900$$

Hence the Solution Vector is:

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.2900 \\ 19.70 \\ 1.050 \end{bmatrix}$$

Finding the inverse of a square matrix

The inverse [B] of a square matrix [*A*] is defined as

$$[A][B] = [I] = [B][A]$$

Finding the inverse of a square matrix

How can LU Decomposition be used to find the inverse?

Assume the first column of [*B*] to be $[b_{11} \;\; b_{12} \;\; \ldots \; b_{n1}]^T$

Using this and the definition of matrix multiplication

First column of [*B*]

$$[A]\begin{bmatrix} b_{11} \\ b_{21} \\ \vdots \\ b_{n1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Second column of [*B*]

$$[A]\begin{bmatrix} b_{12} \\ b_{22} \\ \vdots \\ b_{n2} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

The remaining columns in [*B*] can be found in the same manner

Example: Inverse of a Matrix

Find the inverse of a square matrix [*A*]

$$[A]=\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

Using the decomposition procedure, the [*L*] and [*U*] matrices are found to be

$$[A]=[L][U]=\begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

Example: Inverse of a Matrix

Solving for the each column of [*B*] requires two steps

1) Solve [*L*] [*Z*] = [*C*] for [*Z*]
2) Solve [*U*] [*X*] = [*Z*] for [*X*]

Step 1: $$[L][Z]=[C]\rightarrow\begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}=\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

This generates the equations:

$$z_1 = 1$$

$$2.56z_1 + z_2 = 0$$

$$5.76z_1 + 3.5z_2 + z_3 = 0$$

Example: Inverse of a Matrix

Solving for [Z]

$$
\begin{aligned}
z_1 &= 1 \\
z_2 &= 0 - 2.56 z_1 \\
&= 0 - 2.56(1) \\
&= -2.56 \\
z_3 &= 0 - 5.76 z_1 - 3.5 z_2 \\
&= 0 - 5.76(1) - 3.5(-2.56) \\
&= 3.2
\end{aligned}
$$

$$
[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}
$$

Example: Inverse of a Matrix

Solving [U][X] = [Z] for [X]

$$
\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}
$$

$$
\begin{aligned}
25 b_{11} + 5 b_{21} + b_{31} &= 1 \\
-4.8 b_{21} - 1.56 b_{31} &= -2.56 \\
0.7 b_{31} &= 3.2
\end{aligned}
$$

Example: Inverse of a Matrix

Using Backward Substitution

$$b_{31} = \frac{3.2}{0.7} = 4.571$$

$$b_{21} = \frac{-2.56 + 1.560 b_{31}}{-4.8}$$

$$= \frac{-2.56 + 1.560(4.571)}{-4.8} = -0.9524$$

$$b_{11} = \frac{1 - 5b_{21} - b_{31}}{25}$$

$$= \frac{1 - 5(-0.9524) - 4.571}{25} = 0.04762$$

So the first column of the inverse of [*A*] is:

$$\begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 0.04762 \\ -0.9524 \\ 4.571 \end{bmatrix}$$

Example: Inverse of a Matrix

Repeating for the second and third columns of the inverse

Second Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} -0.08333 \\ 1.417 \\ -5.000 \end{bmatrix}$$

Third Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0.03571 \\ -0.4643 \\ 1.429 \end{bmatrix}$$

Example: Inverse of a Matrix

The inverse of [*A*] is

$$[A]^{-1} = \begin{bmatrix} 0.04762 & -0.08333 & 0.03571 \\ -0.9524 & 1.417 & -0.4643 \\ 4.571 & -5.000 & 1.429 \end{bmatrix}$$

To check your work do the following operation

$$[A][A]^{-1} = [I] = [A]^{-1}[A]$$

THE END

Newton’s Divided Difference Polynomial Method of Interpolation

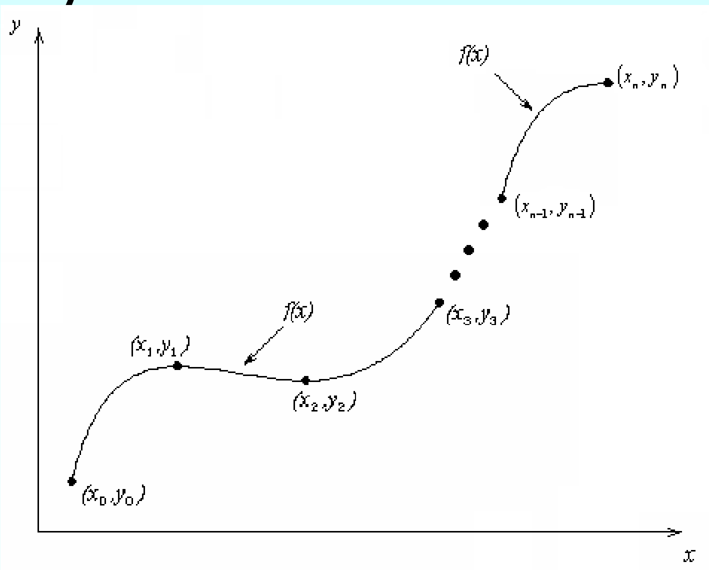
Author: Autar Kaw et. al.

Textbook: TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Newton’s Divided Difference Method of Interpolation

What is Interpolation ?

Given (x_0,y_0), (x_1,y_1), …… ,(x_n,y_n), find the value of 'y' at a value of 'x' that is not given.



What is Interpolation ?

Given (x_0,y_0), (x_1,y_1), …… ,(x_n,y_n), find the value of 'y' at a value of 'x' that is not given.

Interpolation is the process of estimating unknown values that fall between known values

Application: In engineering and science, one often has a function for a limited number of data points. Interpolation is required for finding the function's value at some intermediate points

Interpolants

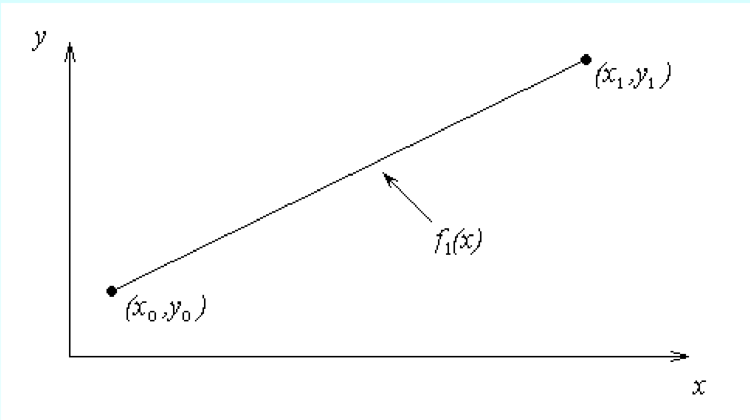
Polynomials are the most common choice of interpolants because they are easy to:

- Evaluate
- Differentiate, and
- Integrate.

Newton's Divided Difference Method

Linear interpolation: Given $(x_0, y_0), (x_1, y_1),$ pass a linear interpolant through the data

$$f_1(x) = b_0 + b_1(x - x_0)$$



where

$$b_0 = f(x_0)$$

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Newton Divided Difference method for linear interpolation.

Table. Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

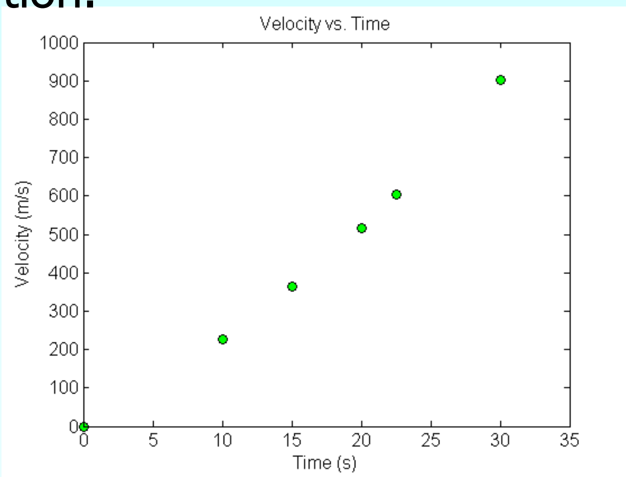


Figure. Velocity vs. time data for the rocket example

Linear Interpolation

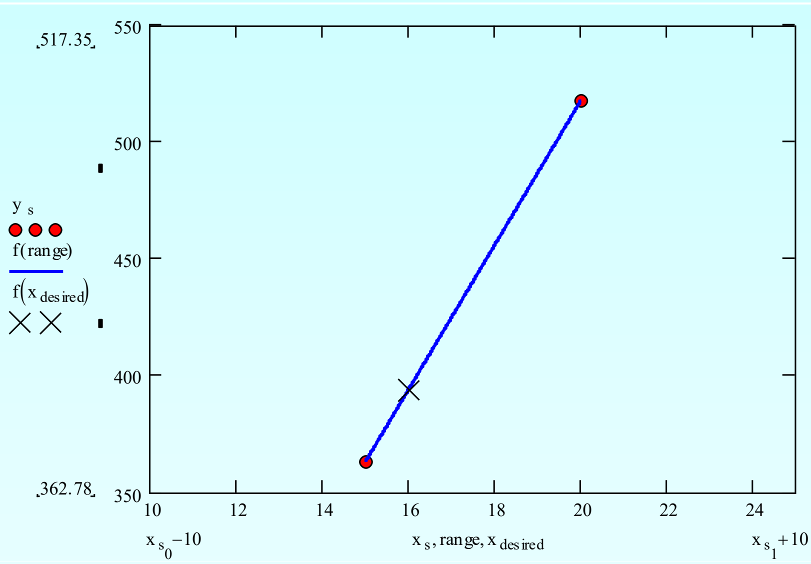
$$v(t) = b_0 + b_1(t - t_0)$$

$$t_0 = 15,\ v(t_0) = 362.78$$

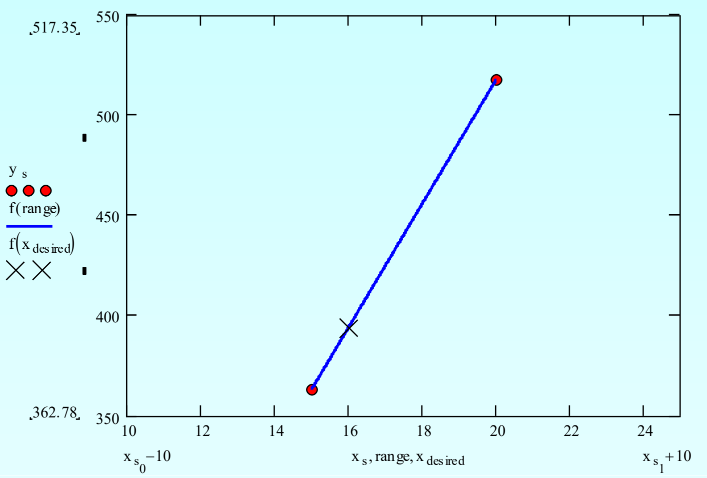
$$t_1 = 20,\ v(t_1) = 517.35$$

$$b_0 = v(t_0) \ = 362.78$$

$$b_1 = \frac{v(t_1) - v(t_0)}{t_1 - t_0} = 30.914$$



Linear Interpolation (contd)



$$v(t) = b_0 + b_1(t - t_0)$$

$$= 362.78 + 30.914(t - 15),\ 15 \le t \le 20$$

At $t = 16$

$$v(16) = 362.78 + 30.914(16 - 15)$$

$$= 393.69 \text{ m/s}$$

Quadratic Interpolation

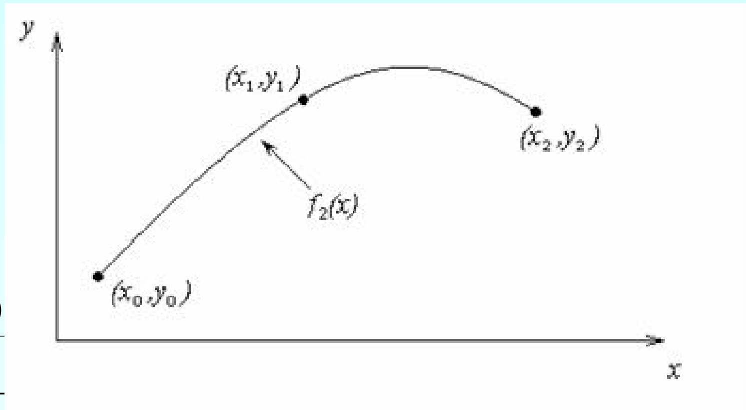
Given (x_0, y_0), (x_1, y_1), and (x_2, y_2), fit a quadratic interpolant through the data.

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

$$b_0 = f(x_0)$$

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$



Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Newton Divided Difference method for quadratic interpolation.

Table. Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

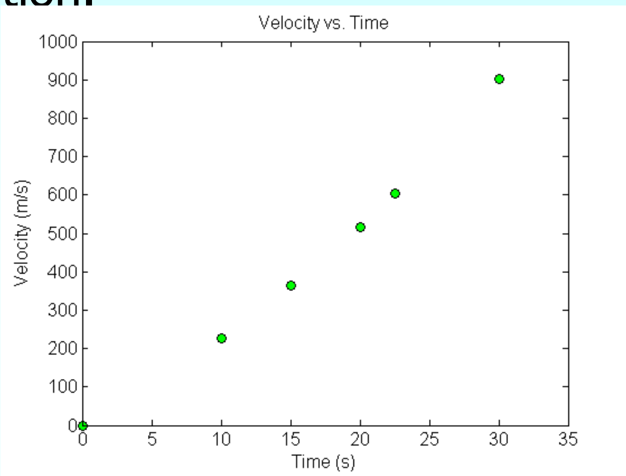
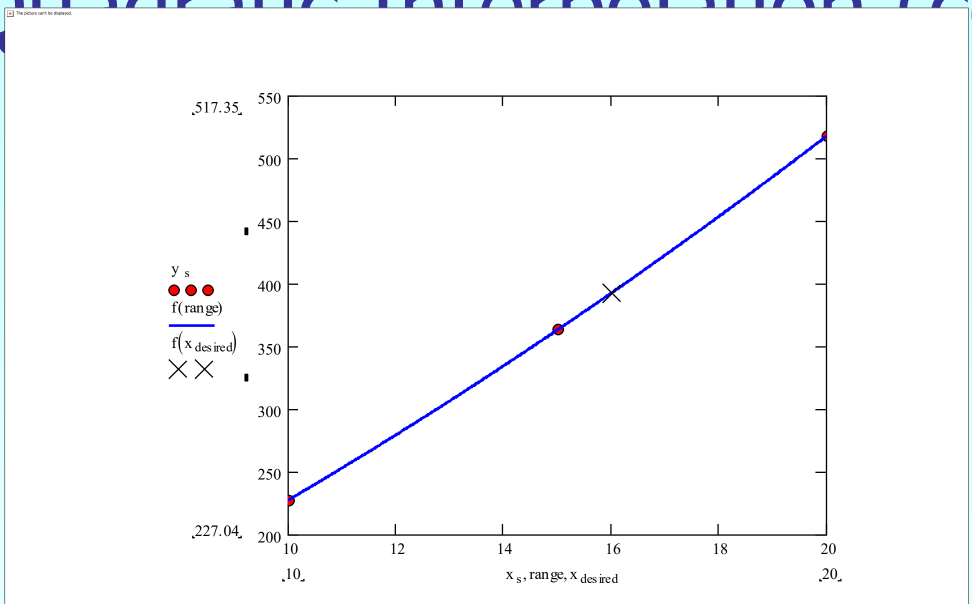


Figure. Velocity vs. time data for the rocket example

Quadratic Interpolation (contd)



$$t_0 = 10, \; v(t_0) = 227.04$$

$$t_1 = 15, \; v(t_1) = 362.78$$

$$t_2 = 20, \; v(t_2) = 517.35$$

Quadratic Interpolation (contd)

$$b_0 = v(t_0)$$
$$= 227.04$$
$$b_1 = \frac{v(t_1) - v(t_0)}{t_1 - t_0} = \frac{362.78 - 227.04}{15 - 10}$$
$$= 27.148$$

$$b_2 = \frac{\dfrac{v(t_2) - v(t_1)}{t_2 - t_1} - \dfrac{v(t_1) - v(t_0)}{t_1 - t_0}}{t_2 - t_0} = \frac{\dfrac{517.35 - 362.78}{20 - 15} - \dfrac{362.78 - 227.04}{15 - 10}}{20 - 10}$$
$$= \frac{30.914 - 27.148}{10}$$
$$= 0.37660$$

Quadratic Interpolation (contd)

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1)$$
$$= 227.04 + 27.148(t - 10) + 0.37660\,(t - 10)(t - 15), \qquad 10 \le t \le 20$$

At $t = 16$,

$$v(16) = 227.04 + 27.148(16 - 10) + 0.37660\,(16 - 10)(16 - 15) = 392.19 \text{ m/s}$$

The absolute relative approximate error $|\in_a|$ obtained between the results from the first order and second order polynomial is

$$|\in_a| = \left|\frac{392.19 - 393.69}{392.19}\right| \text{x} 100$$
$$= 0.38502\ \%$$

General Form

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

where

$$b_0 = f[x_0] = f(x_0)$$

$$b_1 = f[x_1, x_0] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = f[x_2, x_1, x_0] = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0} = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

Rewriting

$$f_2(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1)$$

General Form

Given $(n+1)$ data points, $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$ as

$$f_n(x) = b_0 + b_1(x - x_0) + \ldots. + b_n(x - x_0)(x - x_1)\ldots(x - x_{n-1})$$

where

$$b_0 = f[x_0]$$

$$b_1 = f[x_1, x_0]$$

$$b_2 = f[x_2, x_1, x_0]$$

$$\vdots$$

$$b_{n-1} = f[x_{n-1}, x_{n-2}, \ldots., x_0]$$

$$b_n = f[x_n, x_{n-1}, \ldots., x_0]$$

General form

The third order polynomial, given $(x_0, y_0), (x_1, y_1), (x_2, y_2),$ and $(x_3, y_3),$ is

$$f_3(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1)$$
$$+ f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2)$$

	b_0			
x_0	$f(x_0)$			
		b_1		
		$f[x_1, x_0]$	b_2	
x_1	$f(x_1)$		$f[x_2, x_1, x_0]$	b_3
		$f[x_2, x_1]$		$f[x_3, x_2, x_1, x_0]$
x_2	$f(x_2)$		$f[x_3, x_2, x_1]$	
		$f[x_3, x_2]$		
x_3	$f(x_3)$			

Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Newton Divided Difference method for cubic interpolation.

Table. Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

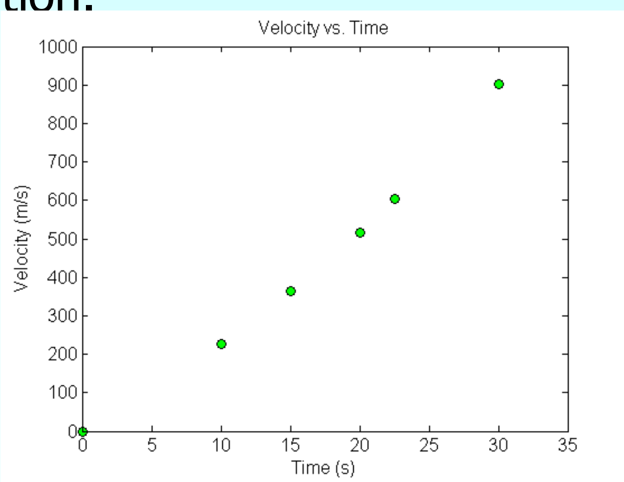


Figure. Velocity vs. time data for the rocket example

Example

The velocity profile is chosen as

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1) + b_3(t - t_0)(t - t_1)(t - t_2)$$

we need to choose four data points that are closest to $t = 16$

$$t_0 = 10, \quad v(t_0) = 227.04$$
$$t_1 = 15, \quad v(t_1) = 362.78$$
$$t_2 = 20, \quad v(t_2) = 517.35$$
$$t_3 = 22.5, \quad v(t_3) = 602.97$$

The values of the constants are found as:

$b_0 = 227.04$; $b_1 = 27.148$; $b_2 = 0.37660$; $b_3 = 5.4347\times10^{-3}$

Example

$t_0 = 10$	227.04 (b_0)			
		27.148 (b_1)		
$t_1 = 15,$	362.78		0.37660 (b_2)	
		30.914		5.4347×10^{-3} (b_3)
$t_2 = 20,$	517.35		0.44453	
		34.248		
$t_3 = 22.5,$	602.97			

$b_0 = 227.04$; $b_1 = 27.148$; $b_2 = 0.37660$; $b_3 = 5.4347\times10^{-3}$

Example

Hence

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1) + b_3(t - t_0)(t - t_1)(t - t_2)$$
$$= 227.04 + 27.148(t - 10) + 0.37660(t - 10)(t - 15)$$
$$+ 5.4347 * 10^{-3}(t - 10)(t - 15)(t - 20)$$

At $t = 16$,

$$v(16) = 227.04 + 27.148(16 - 10) + 0.37660(16 - 10)(16 - 15)$$
$$+ 5.4347 * 10^{-3}(16 - 10)(16 - 15)(16 - 20)$$
$$= 392.06 \text{ m/s}$$

The absolute relative approximate error $|\in_a|$ obtained is

$$|\in_a| = \left|\frac{392.06 - 392.19}{392.06}\right| \text{x}100$$

$$= 0.033427\ \%$$

Comparison Table

Order of Polynomial	1	2	3
v(t=16) m/s	393.69	392.19	392.06
Absolute Relative Approximate Error	----------	0.38502 %	0.033427 %

Distance from Velocity Profile

Find the distance covered by the rocket from t=11s to t=16s ?

$$v(t) = 227.04 + 27.148(t-10) + 0.37660(t-10)(t-15) + 5.4347*10^{-3}(t-10)(t-15)(t-20) \qquad 10 \le t \le 22.5$$

$$= -4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3 \qquad 10 \le t \le 22.5$$

So

$$s(16) - s(11) = \int_{11}^{16} v(t)dt$$

$$= \int_{11}^{16} (-4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3)dt$$

$$= \left[-4.2541t + 21.265\frac{t^2}{2} + 0.13204\frac{t^3}{3} + 0.0054347\frac{t^4}{4}\right]_{11}^{16}$$

$$= 1605\, m$$

Acceleration from Velocity Profile

Find the acceleration of the rocket at t=16s given that

$$v(t) = -4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3$$

$$a(t) = \frac{d}{dt}v(t) = \frac{d}{dt}\left(-4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3\right)$$

$$= 21.265 + 0.26408t + 0.016304t^2$$

$$a(16) = 21.265 + 0.26408(16) + 0.016304(16)^2$$

$$= 29.664\, m/s^2$$

THE END

Lagrangian Interpolation

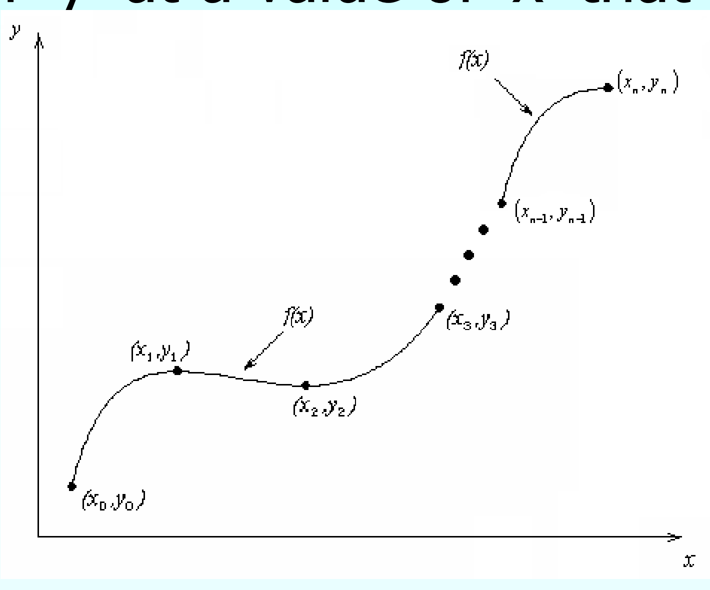
Author: Autar Kaw et. al.

Textbook: TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Lagrange Method of Interpolation

What is Interpolation ?

Given (x_0,y_0), (x_1,y_1), …… (x_n,y_n), find the value of ‘y’ at a value of ‘x’ that is not given.



Interpolants

Polynomials are the most common choice of interpolants because they are easy to:

- Evaluate
- Differentiate, and
- Integrate.

Lagrangian Interpolation

Lagrangian interpolating polynomial is given by

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

where 'n' in $f_n(x)$ stands for the n^{th} order polynomial that approximates the function $y = f(x)$ given at $(n+1)$ data points as $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$, and

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$L_i(x)$ is a weighting function that includes a product of $(n-1)$ terms with terms of $j = i$ omitted.

Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Lagrangian method for linear interpolation.

Table Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

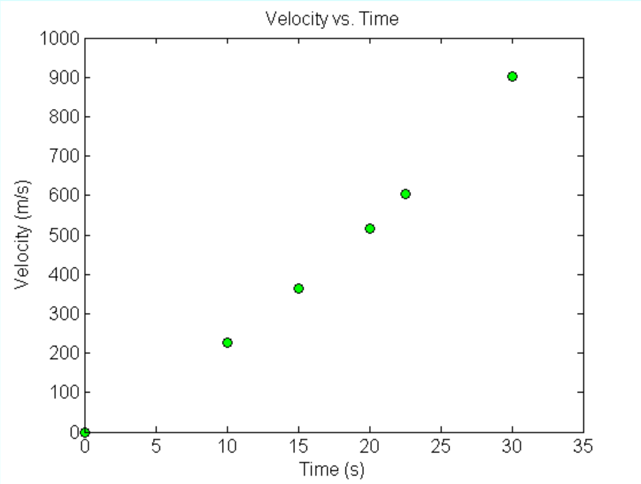


Figure. Velocity vs. time data for the rocket example

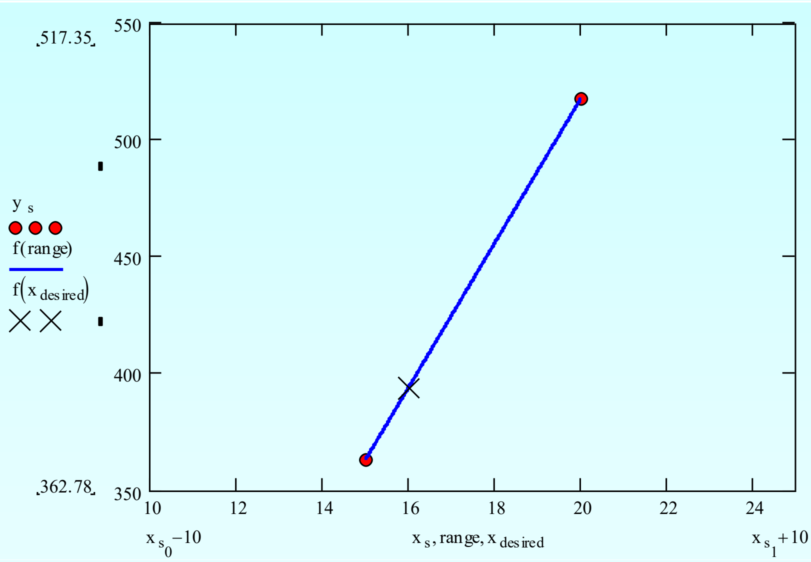
Linear Interpolation

$$v(t) = \sum_{i=0}^{1} L_i(t) v(t_i)$$

$$= L_0(t) v(t_0) + L_1(t) v(t_1)$$

$$t_0 = 15, v(t_0) = 362.78$$

$$t_1 = 20, v(t_1) = 517.35$$



Linear Interpolation (contd)

$$L_0(t) = \prod_{\substack{j=0 \\ j \neq 0}}^{1} \frac{t - t_j}{t_0 - t_j} = \frac{t - t_1}{t_0 - t_1}$$

$$L_1(t) = \prod_{\substack{j=0 \\ j \neq 1}}^{1} \frac{t - t_j}{t_1 - t_j} = \frac{t - t_0}{t_1 - t_0}$$

$$v(t) = \frac{t - t_1}{t_0 - t_1} v(t_0) + \frac{t - t_0}{t_1 - t_0} v(t_1) = \frac{t - 20}{15 - 20}(362.78) + \frac{t - 15}{20 - 15}(517.35)$$

$$v(16) = \frac{16 - 20}{15 - 20}(362.78) + \frac{16 - 15}{20 - 15}(517.35)$$

$$= 0.8(362.78) + 0.2(517.35)$$

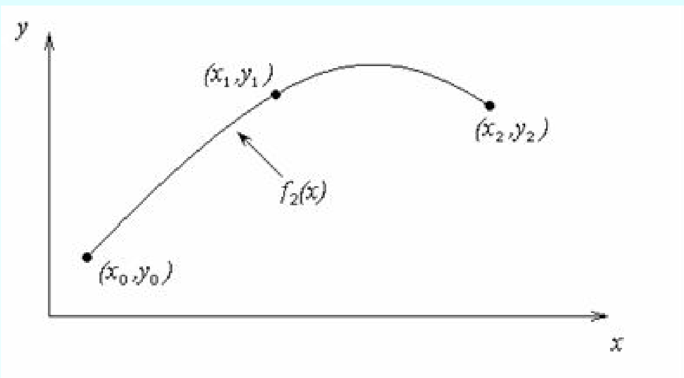
$$= 393.7 \text{ m/s.}$$

Quadratic Interpolation

For the second order polynomial interpolation (also called quadratic interpolation), we choose the velocity given by

$$v(t) = \sum_{i=0}^{2} L_i(t) v(t_i)$$

$$= L_0(t)v(t_0) + L_1(t)v(t_1) + L_2(t)v(t_2)$$



Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Lagrangian method for quadratic interpolation.

Table Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

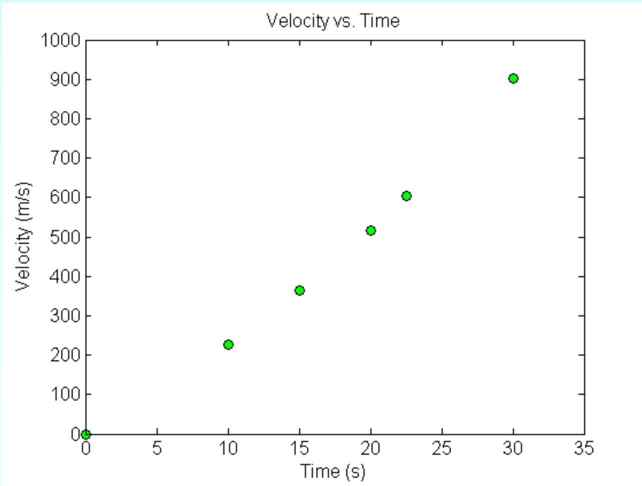


Figure. Velocity vs. time data for the rocket example

Quadratic Interpolation (contd)

$$t_0 = 10,\ v(t_0) = 227.04$$

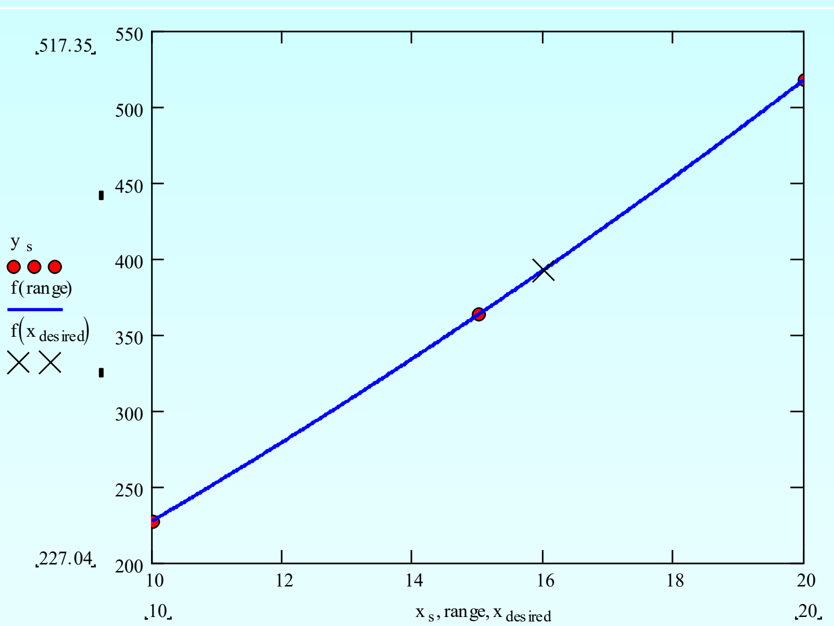
$$t_1 = 15,\ v(t_1) = 362.78$$

$$t_2 = 20,\ v(t_2) = 517.35$$

$$L_0(t) = \prod_{\substack{j=0 \\ j\neq 0}}^{2} \frac{t-t_j}{t_0-t_j} = \left(\frac{t-t_1}{t_0-t_1}\right)\left(\frac{t-t_2}{t_0-t_2}\right)$$

$$L_1(t) = \prod_{\substack{j=0 \\ j\neq 1}}^{2} \frac{t-t_j}{t_1-t_j} = \left(\frac{t-t_0}{t_1-t_0}\right)\left(\frac{t-t_2}{t_1-t_2}\right)$$

$$L_2(t) = \prod_{\substack{j=0 \\ j\neq 2}}^{2} \frac{t-t_j}{t_2-t_j} = \left(\frac{t-t_0}{t_2-t_0}\right)\left(\frac{t-t_1}{t_2-t_1}\right)$$



Quadratic Interpolation (contd)

$$v(t)=\left(\frac{t-t_1}{t_0-t_1}\right)\left(\frac{t-t_2}{t_0-t_2}\right)v(t_0)+\left(\frac{t-t_0}{t_1-t_0}\right)\left(\frac{t-t_2}{t_1-t_2}\right)v(t_1)+\left(\frac{t-t_0}{t_2-t_0}\right)\left(\frac{t-t_1}{t_2-t_1}\right)v(t_2)$$

$$v(16)=\left(\frac{16-15}{10-15}\right)\left(\frac{16-20}{10-20}\right)(227.04)+\left(\frac{16-10}{15-10}\right)\left(\frac{16-20}{15-20}\right)(362.78)+\left(\frac{16-10}{20-10}\right)\left(\frac{16-15}{20-15}\right)(517.35)$$

$$=(-0.08)(227.04)+(0.96)(362.78)+(0.12)(527.35)$$

$$=392.19 \text{ m/s}$$

The absolute relative approximate error $|\in_a|$ obtained between the results from the first and second order polynomial is

$$|\in_a|=\left|\frac{392.19-393.70}{392.19}\right|\times 100$$

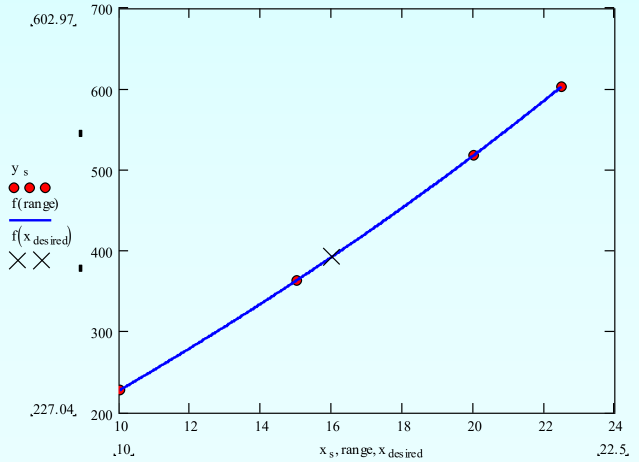
$$=0.38410\%$$

Cubic Interpolation

For the third order polynomial (also called cubic interpolation), we choose the velocity given by

$$v(t)=\sum_{i=0}^{3}L_i(t)v(t_i)$$

$$=L_0(t)v(t_0)+L_1(t)v(t_1)+L_2(t)v(t_2)+L_3(t)v(t_3)$$



Example

The upward velocity of a rocket is given as a function of time in Table 1. Find the velocity at t=16 seconds using the Lagrangian method for cubic interpolation.

Table Velocity as a function of time

t (s)	$v(t)$ (m/s)
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

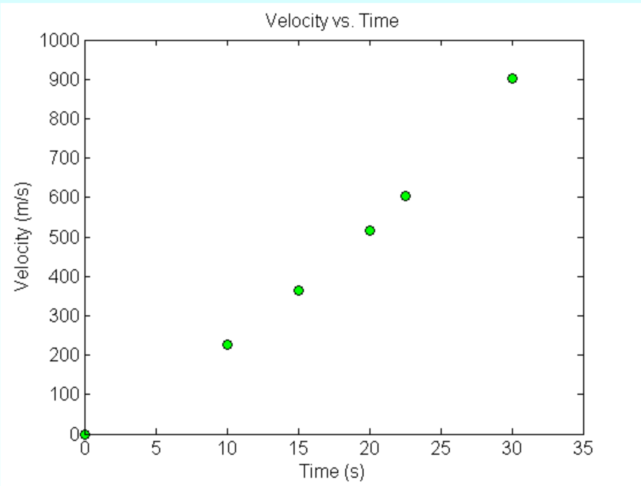


Figure. Velocity vs. time data for the rocket example

Cubic Interpolation (contd)

$t_o = 10,\ v(t_o) = 227.04 \qquad t_1 = 15,\ v(t_1) = 362.78$

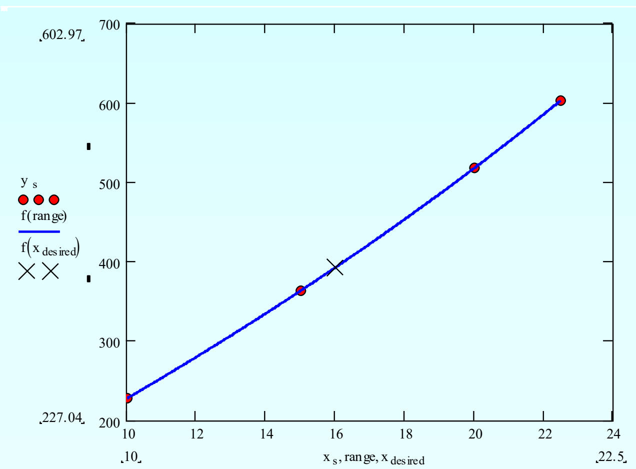
$t_2 = 20,\ v(t_2) = 517.35 \qquad t_3 = 22.5,\ v(t_3) = 602.97$

$$L_0(t) = \prod_{\substack{j=0 \\ j\neq 0}}^{3} \frac{t-t_j}{t_0-t_j} = \left(\frac{t-t_1}{t_0-t_1}\right)\left(\frac{t-t_2}{t_0-t_2}\right)\left(\frac{t-t_3}{t_0-t_3}\right);$$

$$L_1(t) = \prod_{\substack{j=0 \\ j\neq 1}}^{3} \frac{t-t_j}{t_1-t_j} = \left(\frac{t-t_0}{t_1-t_0}\right)\left(\frac{t-t_2}{t_1-t_2}\right)\left(\frac{t-t_3}{t_1-t_3}\right)$$

$$L_2(t) = \prod_{\substack{j=0 \\ j\neq 2}}^{3} \frac{t-t_j}{t_2-t_j} = \left(\frac{t-t_0}{t_2-t_0}\right)\left(\frac{t-t_1}{t_2-t_1}\right)\left(\frac{t-t_3}{t_2-t_3}\right);$$

$$L_3(t) = \prod_{\substack{j=0 \\ j\neq 3}}^{3} \frac{t-t_j}{t_3-t_j} = \left(\frac{t-t_0}{t_3-t_0}\right)\left(\frac{t-t_1}{t_3-t_1}\right)\left(\frac{t-t_2}{t_3-t_2}\right)$$



Cubic Interpolation (contd)

$$v(t)=\left(\frac{t-t_1}{t_0-t_1}\right)\left(\frac{t-t_2}{t_0-t_2}\right)\left(\frac{t-t_3}{t_0-t_3}\right)v(t_1)+\left(\frac{t-t_0}{t_1-t_0}\right)\left(\frac{t-t_2}{t_1-t_2}\right)\left(\frac{t-t_3}{t_1-t_3}\right)v(t_2)$$

$$+\left(\frac{t-t_0}{t_2-t_0}\right)\left(\frac{t-t_1}{t_2-t_1}\right)\left(\frac{t-t_3}{t_2-t_3}\right)v(t_2)+\left(\frac{t-t_1}{t_3-t_1}\right)\left(\frac{t-t_1}{t_3-t_1}\right)\left(\frac{t-t_2}{t_3-t_2}\right)v(t_3)$$

$$v(16)=\left(\frac{16-15}{10-15}\right)\left(\frac{16-20}{10-20}\right)\left(\frac{16-22.5}{10-22.5}\right)(227.04)+\left(\frac{16-10}{15-10}\right)\left(\frac{16-20}{15-20}\right)\left(\frac{16-22.5}{15-22.5}\right)(362.78)$$

$$+\left(\frac{16-10}{20-10}\right)\left(\frac{16-15}{20-15}\right)\left(\frac{16-22.5}{20-22.5}\right)(517.35)+\left(\frac{16-10}{22.5-10}\right)\left(\frac{16-15}{22.5-15}\right)\left(\frac{16-20}{22.5-20}\right)(602.97)$$

$$=(-0.0416)(227.04)+(0.832)(362.78)+(0.312)(517.35)+(-0.1024)(602.97)$$

$$=392.06\,\mathrm{m/s}$$

The absolute relative approximate error $|\in_a|$ obtained between the results from the first and second order polynomial is

$$|\in_a|=\left|\frac{392.06-392.19}{392.06}\right|\times 100$$

$$=0.033269\%$$

Comparison Table

Order of Polynomial	**1**	**2**	**3**
v(t=16) m/s	393.69	392.19	392.06
Absolute Relative Approximate Error	--------	0.38410%	0.033269%

Distance from Velocity Profile

Find the distance covered by the rocket from t=11s to t=16s ?

$$v(t) = (t^3 - 57.5t^2 + 1087.5t - 6750)(-0.36326) + (t^3 - 52.5t^2 + 875t - 4500)(1.9348)$$
$$+ (t^3 - 47.5t^2 + 712.5t - 3375)(-4.1388) + (t^3 - 45t^2 + 650t - 3000)(2.5727)$$

$$v(t) = -4.245 + 21.265t + 0.13195t^2 + 0.00544t^3, \quad 10 \le t \le 22.5$$

$$s(16) - s(11) = \int_{11}^{16} v(t)dt$$

$$\approx \int_{11}^{16} (-4.245 + 21.265t + 0.13195t^2 + 0.00544t^3)dt$$

$$= [-4.245t + 21.265\frac{t^2}{2} + 0.13195\frac{t^3}{3} + 0.00544\frac{t^4}{4}]_{11}^{16}$$

$$= 1605 \ \text{m}$$

Acceleration from Velocity Profile

Find the acceleration of the rocket at t=16s given that

$$v(t) = -4.245 + 21.265t + 0.13195t^2 + 0.00544t^3, \quad 10 \le t \le 22.5$$

$$a(t) = \frac{d}{dt}v(t) = \frac{d}{dt}\left(-4.245 + 21.265t + 0.13195t^2 + 0.00544t^3\right)$$

$$= 21.265 + 0.26390t + 0.01632t^2$$

$$a(16) = 21.265 + 0.26390(16) + 0.01632(16)^2$$

$$= 29.665 \ \ m/s^2$$

THE END

Integration

Author: Autar Kaw et. al.

Textbook: TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Trapezoidal Rule of Integration

What is Integration

Integration:

The process of measuring the area under a function plotted on a graph.

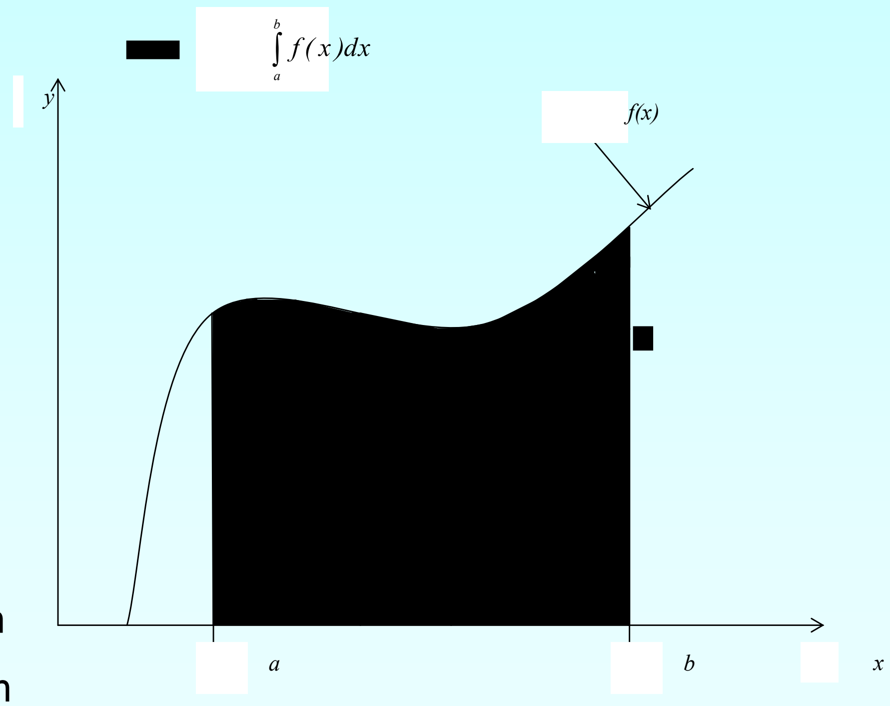
$$I = \int_a^b f(x)dx$$

Where:

f(x) is the integrand

a= lower limit of integration

b= upper limit of integration



Basis of Trapezoidal Rule

Trapezoidal Rule is based on the Newton-Cotes Formula that states if one can approximate the integrand as an n^{th} order polynomial…

$I = \int_a^b f(x)dx$ where $f(x) \approx f_n(x)$

and $f_n(x) = a_0 + a_1 x + ... + a_{n-1}x^{n-1} + a_n x^n$

Basis of Trapezoidal Rule

Then the integral of that function is approximated by the integral of that n^{th} order polynomial.

$$\int_a^b f(x) \approx \int_a^b f_n(x)$$

Trapezoidal Rule assumes n=1, that is, the area under the linear polynomial,

$$\int_a^b f(x)dx = (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

Derivation of the Trapezoidal Rule

Method Derived From Geometry

The area under the curve is a trapezoid. The integral

$$\int_a^b f(x)dx \approx Area\ of\ trapezoid$$

$$= \frac{1}{2}(Sum\ of\ parallel\ sides)(height)$$

$$= \frac{1}{2}(f(b)+f(a))(b-a)$$

$$= (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

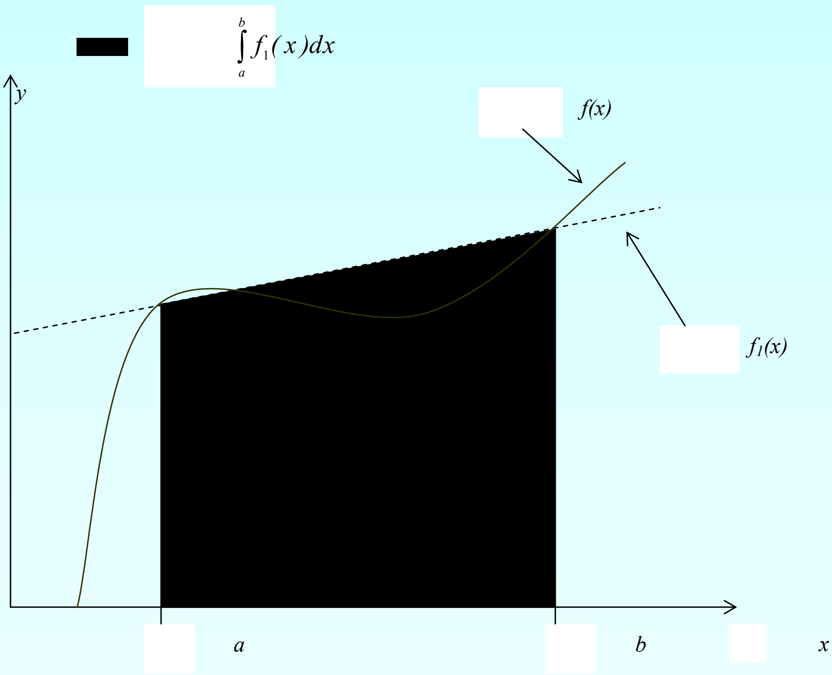


Figure 2: Geometric Representation

Example 1

The vertical distance covered by a rocket from t=8 to t=30 seconds is given by:

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use single segment Trapezoidal rule to find the distance covered.
b) Find the true error, E_t for part (a).
c) Find the absolute relative true error, $|\in_a|$ for part (a).

Solution

a) $$I \approx (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

$a = 8 \qquad b = 30$

$$f(t) = 2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t$$

$$f(8) = 2000 \ln \left[\frac{140000}{140000 - 2100(8)} \right] - 9.8(8) \quad = 177.27 \ m/s$$

$$f(30) = 2000 \ln \left[\frac{140000}{140000 - 2100(30)} \right] - 9.8(30) \quad = 901.67 \ m/s$$

Solution (cont)

a) $$I = (30-8)\left[\frac{177.27+901.67}{2}\right]$$

$$= 11868\ m$$

b) The exact value of the above integral is

$$x = \int_8^{30}\left(2000\,ln\left[\frac{140000}{140000-2100t}\right]-9.8t\right)dt \quad = 11061\ m$$

Solution (cont)

b) $$E_t = True\ Value - Approximate\ Value$$

$$= 11061 - 11868$$

$$= -807\ m$$

c) The absolute relative true error, $|\in_t|$, would be

$$|\in_t| = \left|\frac{11061-11868}{11061}\right| \times 100 = 7.2959\%$$

Multiple Segment Trapezoidal Rule

In Example 1, the true error using single segment trapezoidal rule was large. We can divide the interval [8,30] into [8,19] and [19,30] intervals and apply Trapezoidal rule over each segment.

$$f(t) = 2000 ln\left(\frac{140000}{140000-2100t}\right) - 9.8t$$

$$\int_{8}^{30} f(t)dt = \int_{8}^{19} f(t)dt + \int_{19}^{30} f(t)dt$$

$$= (19-8)\left[\frac{f(8)+f(19)}{2}\right] + (30-19)\left[\frac{f(19)+f(30)}{2}\right]$$

Multiple Segment Trapezoidal Rule

With

$$f(8) = 177.27 \ m/s$$

$$f(30) = 901.67 \ m/s$$

$$f(19) = 484.75 \ m/s$$

Hence:

$$\int_{8}^{30} f(t)dt = (19-8)\left[\frac{177.27+484.75}{2}\right] + (30-19)\left[\frac{484.75+901.67}{2}\right]$$

$$= 11266 \ m$$

Multiple Segment Trapezoidal Rule

The true error is:

$$E_t = 11061 - 11266$$
$$= -205\ m$$

The true error now is reduced from -807 m to -205 m.

Extending this procedure to divide the interval into equal segments to apply the Trapezoidal rule; the sum of the results obtained for each segment is the approximate value of the integral.

Multiple Segment Trapezoidal Rule

Divide into equal segments as shown in Figure 4. Then the width of each segment is:

$$h = \frac{b-a}{n}$$

The integral I is:

$$I = \int_a^b f(x)dx$$

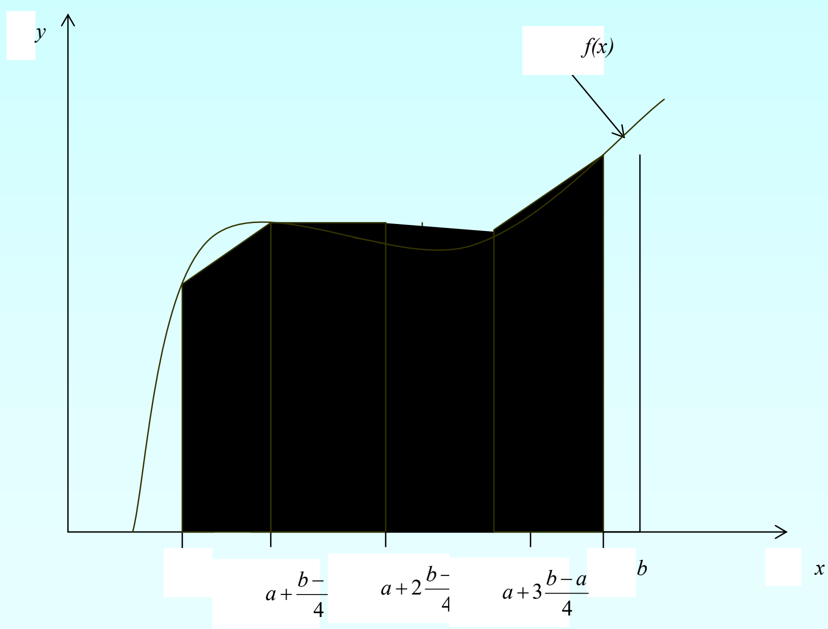


Figure 4: Multiple (n=4) Segment Trapezoidal Rule

Multiple Segment Trapezoidal Rule

The integral I can be broken into h integrals as:

$$\int_a^b f(x)dx = \int_a^{a+h} f(x)dx + \int_{a+h}^{a+2h} f(x)dx + \ldots + \int_{a+(n-2)h}^{a+(n-1)h} f(x)dx + \int_{a+(n-1)h}^{b} f(x)dx$$

Applying Trapezoidal rule on each segment gives:

$$\int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a) + 2\left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right]$$

Example 2

The vertical distance covered by a rocket from to seconds is given by:

$$x = \int_8^{30} \left(2000 ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use two-segment Trapezoidal rule to find the distance covered.
b) Find the true error, E_t for part (a).
c) Find the absolute relative true error, $|\in_a|$ for part (a).

Solution

a) The solution using 2-segment Trapezoidal rule is

$$I = \frac{b-a}{2n}\left[f(a) + 2\left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right]$$

$$n = 2 \qquad a = 8 \qquad b = 30$$

$$h = \frac{b-a}{n} = \frac{30-8}{2} = 11$$

Solution (cont)

Then:

$$I = \frac{30-8}{2(2)}\left[f(8) + 2\left\{ \sum_{i=1}^{2-1} f(a+ih) \right\} + f(30) \right]$$

$$= \frac{22}{4}\left[f(8) + 2f(19) + f(30) \right]$$

$$= \frac{22}{4}\left[177.27 + 2(484.75) + 901.67 \right]$$

$$= 11266 \ m$$

Solution (cont)

b) The exact value of the above integral is

$$x = \int_{8}^{30} \left(2000\, ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt \quad = 11061\ m$$

so the true error is

$$E_t = True\ Value - Approximate\ Value$$

$$= 11061 - 11266$$

Solution (cont)

The absolute relative true error, $\left|\in_t\right|$, would be

$$\left|\in_t\right| = \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100$$

$$= \left| \frac{11061 - 11266}{11061} \right| \times 100$$

$$= 1.8534\%$$

Solution (cont)

Table 1 gives the values obtained using multiple segment Trapezoidal rule for

$$x = \int_8^{30} \left(2000 \ln\left[\frac{140000}{140000 - 2100t}\right] - 9.8t \right) dt$$

Exact Value=11061 m

n	Value	E_t	$\left\|\in_t\right\|\%$	$\left\|\in_a\right\|\%$
1	11868	-807	7.296	---
2	11266	-205	1.853	5.343
3	11153	-91.4	0.8265	1.019
4	11113	-51.5	0.4655	0.3594
5	11094	-33.0	0.2981	0.1669
6	11084	-22.9	0.2070	0.09082
7	11078	-16.8	0.1521	0.05482
8	11074	-12.9	0.1165	0.03560

Table 1: Multiple Segment Trapezoidal Rule Values

Example 3

Use Multiple Segment Trapezoidal Rule to find the area under the curve

$$f(x) = \frac{300x}{1+e^x}$$ from $x = 0$ to $x = 10$

Using two segments, we get $h = \frac{10-0}{2} = 5$ and

$$f(0) = \frac{300(0)}{1+e^0} = 0 \qquad f(5) = \frac{300(5)}{1+e^5} = 10.039 \qquad f(10) = \frac{300(10)}{1+e^{10}} = 0.136$$

Solution

Then:

$$I=\frac{b-a}{2n}\left[f(a)+2\left\{\sum_{i=1}^{n-1}f(a+ih)\right\}+f(b)\right]$$

$$=\frac{10-0}{2(2)}\left[f(0)+2\left\{\sum_{i=1}^{2-1}f(0+5)\right\}+f(10)\right]$$

$$=\frac{10}{4}\left[f(0)+2f(5)+f(10)\right]=\frac{10}{4}\left[0+2(10.039)+0.136\right]$$

$$=50.535$$

Solution (cont)

So what is the true value of this integral?

$$\int_0^{10}\frac{300x}{1+e^x}dx=246.59$$

Making the absolute relative true error:

$$\left|\in_t\right|=\left|\frac{246.59-50.535}{246.59}\right|\times 100\%$$

$$=79.506\%$$

Solution (cont)

Table 2: Values obtained using Multiple Segment Trapezoidal Rule for: $\int_0^{10} \frac{300x}{1+e^x}dx$

n	Approximate Value	E_t	$\lvert \in_t \rvert$
1	0.681	245.91	99.724%
2	50.535	196.05	79.505%
4	170.61	75.978	30.812%
8	227.04	19.546	7.927%
16	241.70	4.887	1.982%
32	245.37	1.222	0.495%
64	246.28	0.305	0.124%

Error in Multiple Segment Trapezoidal Rule

The true error for a single segment Trapezoidal rule is given by:

$E_t = \frac{(b-a)^3}{12} f''(\zeta), \quad a < \zeta < b$ where ζ is some point in $[a,b]$

What is the error, then in the multiple segment Trapezoidal rule? It will be simply the sum of the errors from each segment, where the error in each segment is that of the single segment Trapezoidal rule.

The error in each segment is

$$E_1 = \frac{[(a+h)-a]^3}{12} f''(\zeta_1), \quad a < \zeta_1 < a+h$$

$$= \frac{h^3}{12} f''(\zeta_1)$$

Error in Multiple Segment Trapezoidal Rule

Similarly:

$$E_i = \frac{[(a+ih)-(a+(i-1)h)]^3}{12} f''(\zeta_i), \quad a+(i-1)h < \zeta_i < a+ih$$

$$= \frac{h^3}{12} f''(\zeta_i)$$

It then follows that:

$$E_n = \frac{[b-\{a+(n-1)h\}]^3}{12} f''(\zeta_n), \quad a+(n-1)h < \zeta_n < b$$

$$= \frac{h^3}{12} f''(\zeta_n)$$

Error in Multiple Segment Trapezoidal Rule

Hence the total error in multiple segment Trapezoidal rule is

$$E_t = \sum_{i=1}^{n} E_i \qquad = \frac{h^3}{12}\sum_{i=1}^{n} f''(\zeta_i) \quad = \frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$$

The term $\dfrac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$ is an approximate average value of the $f''(x),\ a < x < b$

Hence:

$$E_t = \frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^{n} f''(\zeta_i)}{n}$$

Error in Multiple Segment Trapezoidal Rule

Below is the table for the integral $\int_{8}^{30}\left(2000\,ln\left[\frac{140000}{140000-2100t}\right]-9.8t\right)dt$

as a function of the number of segments. You can visualize that as the number of segments are doubled, the true error gets approximately quartered.

n	**Value**	E_t	$\lvert\in_t\rvert\%$	$\lvert\in_a\rvert\%$
2	11266	-205	1.854	5.343
4	11113	-51.5	0.4655	0.3594
8	11074	-12.9	0.1165	0.03560
16	11065	-3.22	0.02913	0.00401

THE END

Simpson's 1/3rd Rule of Integration

Author: Autar Kaw et. al.

Textbook: TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Simpson's 1/3rd Rule of Integration

What is Integration?

Integration

The process of measuring the area under a curve.

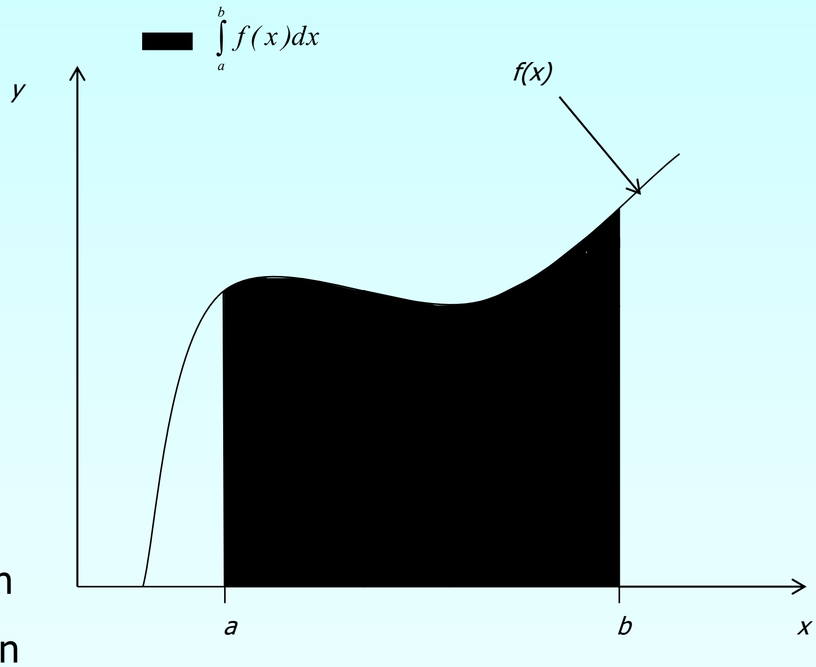
$$I = \int_a^b f(x)dx$$

Where:

f(x) is the integrand

a= lower limit of integration

b= upper limit of integration



Simpson's 1/3rd Rule

Basis of Simpson’s 1/3rd Rule

Trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial in the interval of integration. Simpson’s 1/3rd rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

Hence

$$I = \int_a^b f(x)dx \approx \int_a^b f_2(x)dx$$

Where $f_2(x)$ is a second order polynomial.

$$f_2(x) = a_0 + a_1 x + a_2 x^2$$

Basis of Simpson’s 1/3rd Rule

Choose

$(a, f(a)),\ \left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right),$ and $(b, f(b))$

as the three points of the function to evaluate a_0, a_1 and a_2.

$$f(a) = f_2(a) = a_0 + a_1 a + a_2 a^2$$

$$f\left(\frac{a+b}{2}\right) = f_2\left(\frac{a+b}{2}\right) = a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2$$

$$f(b) = f_2(b) = a_0 + a_1 b + a_2 b^2$$

Basis of Simpson's 1/3rd Rule

Solving the previous equations for a_0, a_1 and a_2 give

$$a_0 = \frac{a^2 f(b) + abf(b) - 4abf\left(\frac{a+b}{2}\right) + abf(a) + b^2 f(a)}{a^2 - 2ab + b^2}$$

$$a_1 = -\frac{af(a) - 4af\left(\frac{a+b}{2}\right) + 3af(b) + 3bf(a) - 4bf\left(\frac{a+b}{2}\right) + bf(b)}{a^2 - 2ab + b^2}$$

$$a_2 = \frac{2\left(f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right)}{a^2 - 2ab + b^2}$$

Basis of Simpson's 1/3rd Rule

Then

$$I \approx \int_a^b f_2(x)dx$$

$$= \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3}\right]_a^b$$

$$= a_0(b-a) + a_1 \frac{b^2 - a^2}{2} + a_2 \frac{b^3 - a^3}{3}$$

Basis of Simpson's 1/3rd Rule

Substituting values of a_0, a_1, a_2 give

$$\int_a^b f_2(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Since for Simpson's 1/3rd Rule, the interval [a, b] is broken into 2 segments, the segment width

$$h = \frac{b-a}{2}$$

Basis of Simpson's 1/3rd Rule

Hence

$$\int_a^b f_2(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Because the above form has 1/3 in its formula, it is called Simpson's 1/3rd Rule.

Example 1

The distance covered by a rocket from t=8 to t=30 is given by

$$x = \int_{8}^{30} \left(2000\, ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use Simpson's 1/3rd Rule to find the approximate value of x

b) Find the true error, E_t

c) Find the absolute relative true error, $|\in_t|$

Solution

a)

$$x = \int_{8}^{30} f(t)dt$$

$$x = \left(\frac{b-a}{6} \right) \left[f(a) + 4f\left(\frac{a+b}{2} \right) + f(b) \right]$$

$$= \left(\frac{30-8}{6} \right) [f(8) + 4f(19) + f(30)]$$

$$= \left(\frac{22}{6} \right) [177.2667 + 4(484.7455) + 901.6740]$$

$$= 11065.72\ m$$

Solution (cont)

b) The exact value of the above integral is

$$x = \int_{8}^{30}\left(2000\,ln\left[\frac{140000}{140000-2100t}\right]-9.8t\right)dt$$

$$= 11061.34\ m$$

True Error

$$E_t = 11061.34 - 11065.72$$

$$= -4.38\ m$$

Solution (cont)

a)c) Absolute relative true error,

$$\left|\in_t\right| = \left|\frac{11061.34-11065.72}{11061.34}\right|\times 100\%$$

$$= 0.0396\%$$

Multiple Segment Simpson's 1/3rd Rule

Multiple Segment Simpson's 1/3rd Rule

Just like in multiple segment Trapezoidal Rule, one can subdivide the interval [a, b] into n segments and apply Simpson's 1/3rd Rule repeatedly over every two segments. Note that n needs to be even. Divide interval [a, b] into equal segments, hence the segment width

$$h = \frac{b-a}{n} \qquad \int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$

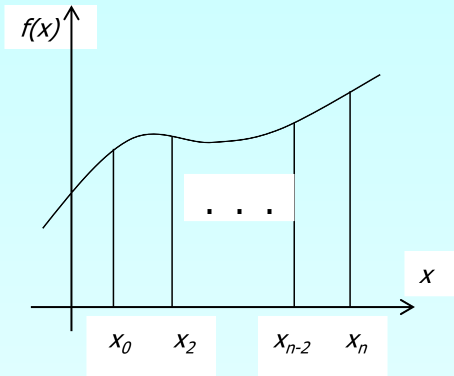
where

$$x_0 = a \qquad x_n = b$$

Multiple Segment Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots..$$

$$\ldots. + \int_{x_{n-4}}^{x_{n-2}} f(x)dx + \int_{x_{n-2}}^{x_n} f(x)dx$$



Apply Simpson's 1/3rd Rule over each interval,

$$\int_a^b f(x)dx = (x_2 - x_0)\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + \ldots$$

$$+ (x_4 - x_2)\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + \ldots$$

Multiple Segment Simpson's 1/3rd Rule

$$\ldots + (x_{n-2} - x_{n-4})\left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6}\right] + \ldots$$

$$+ (x_n - x_{n-2})\left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}\right]$$

Since

$$x_i - x_{i-2} = 2h \qquad i = 2, 4, \ldots, n$$

Multiple Segment Simpson's 1/3rd Rule

Then

$$\int_a^b f(x)dx = 2h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_2)+4f(x_3)+f(x_4)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-4})+4f(x_{n-3})+f(x_{n-2})}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right]$$

Multiple Segment Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \frac{h}{3}[f(x_0)+4\{f(x_1)+f(x_3)+\ldots+f(x_{n-1})\}+\ldots]$$

$$\ldots+2\{f(x_2)+f(x_4)+\ldots+f(x_{n-2})\}+f(x_n)\}]$$

$$=\frac{h}{3}\left[f(x_0)+4\sum_{\substack{i=1\\i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\i=even}}^{n-2}f(x_i)+f(x_n)\right]$$

$$=\frac{b-a}{3n}\left[f(x_0)+4\sum_{\substack{i=1\\i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\i=even}}^{n-2}f(x_i)+f(x_n)\right]$$

Example 2

Use 4-segment Simpson's 1/3rd Rule to approximate the distance

covered by a rocket from t= 8 to t=30 as given by

$$x = \int_{8}^{30} \left(2000 \ln\left[\frac{140000}{140000 - 2100t}\right] - 9.8t \right) dt$$

a) Use four segment Simpson's 1/3rd Rule to find the approximate value of *x*.

b) Find the true error, E_t for part (a).

c) Find the absolute relative true error, $|\in_a|$ for part (a).

Solution

a) Using n segment Simpson's 1/3rd Rule,

$$h = \frac{30-8}{4} = 5.5$$

So

$$f(t_0) = f(8)$$

$$f(t_1) = f(8+5.5) = f(13.5)$$

$$f(t_2) = f(13.5+5.5) = f(19)$$

$$f(t_3) = f(19+5.5) = f(24.5)$$

$$f(t_4) = f(30)$$

Solution (cont.)

$$x = \frac{b-a}{3n}\left[f(t_0) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(t_i) + f(t_n) \right]$$

$$= \frac{30-8}{3(4)}\left[f(8) + 4\sum_{\substack{i=1 \\ i=odd}}^{3} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{2} f(t_i) + f(30) \right]$$

$$= \frac{22}{12}\left[f(8) + 4f(t_1) + 4f(t_3) + 2f(t_2) + f(30) \right]$$

Solution (cont.)

cont.

$$= \frac{11}{6}\left[f(8) + 4f(13.5) + 4f(24.5) + 2f(19) + f(30) \right]$$

$$= \frac{11}{6}\left[177.2667 + 4(320.2469) + 4(676.0501) + 2(484.7455) + 901.6740 \right]$$

$$= 11061.64\ m$$

Solution (cont.)

b) In this case, the true error is

$$E_t = 11061.34 - 11061.64 = -0.30\ m$$

c) The absolute relative true error

$$\left|\in_t\right| = \left|\frac{11061.34 - 11061.64}{11061.34}\right| \times 100\%$$

$$= 0.0027\%$$

Solution (cont.)

Table 1: Values of Simpson's 1/3rd Rule for Example 2 with multiple segments

n	Approximate Value	E_t	$\lvert\in_t\rvert$
2	11065.72	4.38	0.0396%
4	11061.64	0.30	0.0027%
6	11061.40	0.06	0.0005%
8	11061.35	0.01	0.0001%
10	11061.34	0.00	0.0000%

Error in the Multiple Segment Simpson's 1/3rd Rule

The true error in a single application of Simpson's 1/3rd Rule is given as

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta), \quad a < \zeta < b$$

In Multiple Segment Simpson's 1/3rd Rule, the error is the sum of the errors in each application of Simpson's 1/3rd Rule. The error in n segment Simpson's 1/3rd Rule is given by

$$E_1 = -\frac{(x_2 - x_0)^5}{2880} f^{(4)}(\zeta_1) = -\frac{h^5}{90} f^{(4)}(\zeta_1), \quad x_0 < \zeta_1 < x_2$$

$$E_2 = -\frac{(x_4 - x_2)^5}{2880} f^{(4)}(\zeta_2) = -\frac{h^5}{90} f^{(4)}(\zeta_2), \quad x_2 < \zeta_2 < x_4$$

Error in the Multiple Segment Simpson's 1/3rd Rule

$$E_i = -\frac{(x_{2i} - x_{2(i-1)})^5}{2880} f^{(4)}(\zeta_i) = -\frac{h^5}{90} f^{(4)}(\zeta_i), \quad x_{2(i-1)} < \zeta_i < x_{2i}$$

.

.

.

$$E_{\frac{n}{2}-1} = -\frac{(x_{n-2} - x_{n-4})^5}{2880} f^{(4)}\left(\zeta_{\frac{n}{2}-1}\right) = -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}-1}\right), \quad x_{n-4} < \zeta_{\frac{n}{2}-1} < x_{n-2}$$

$$E_{\frac{n}{2}} = -\frac{(x_n - x_{n-2})^5}{2880} f^{4}\left(\zeta_{\frac{n}{2}}\right) = -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}}\right), \quad x_{n-2} < \zeta_{\frac{n}{2}} < x_n$$

Error in the Multiple Segment Simpson's 1/3rd Rule

Hence, the total error in Multiple Segment Simpson's 1/3rd Rule is

$$E_t = \sum_{i=1}^{\frac{n}{2}} E_i \quad = -\frac{h^5}{90}\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i) \quad = -\frac{(b-a)^5}{90n^5}\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)$$

$$= -\frac{(b-a)^5}{90n^4}\frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$$

Error in the Multiple Segment Simpson's 1/3rd Rule

The term $\dfrac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$ is an approximate average value of

$$f^{(4)}(x),\ a < x < b$$

Hence

$$E_t = -\frac{(b-a)^5}{90n^4}\overline{f}^{(4)}$$

where

$$\overline{f}^{(4)} = \frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$$

THE END

Linear Regression

Author: Autar Kaw et. al.

Textbook: TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Linear Regression

What is Regression?

What is regression? Given n data points $(x_1, y_1), (x_2, y_2), \ldots\ldots, (x_n, y_n)$ best fit $y = f(x)$ to the data.

Residual at each point is $E_i = y_i - f(x_i)$

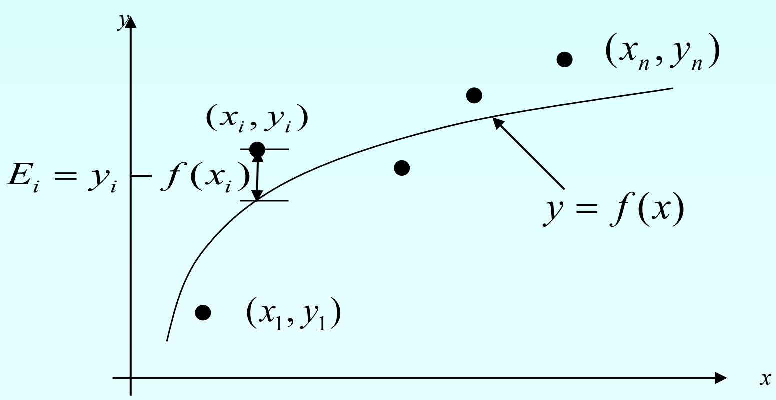


Figure. Basic model for regression

Linear Regression-Criterion#1

Given n data points $(x_1, y_1), (x_2, y_2), \ldots\ldots, (x_n, y_n)$ best fit $y = a_0 + a_1 x$ to the data.

Does minimizing $\sum_{i=1}^{n} E_i$ work as a criterion?

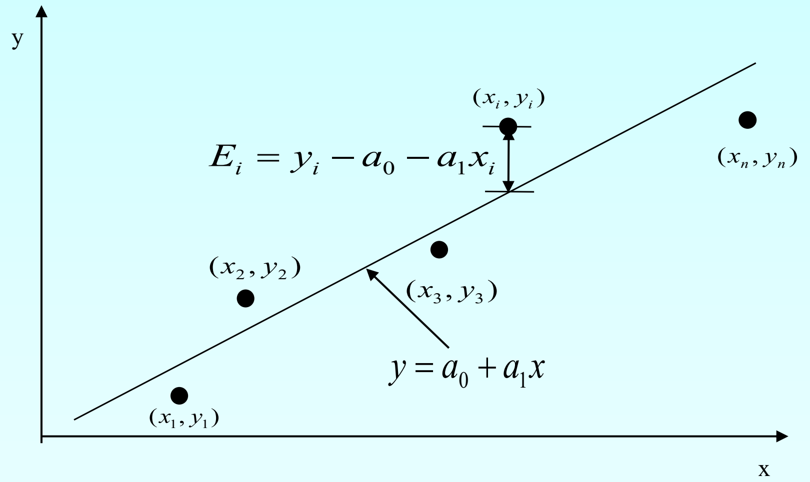


Figure. Linear regression of y vs x data showing residuals at a typical point, x_i .

Example for Criterion#1

Example: Given the data points (2,4), (3,6), (2,6) and (3,8), best fit the data to a straight line using Criterion#1

Minimize $\sum_{i=1}^{n} E_i$

Table. Data Points

x	y
2.0	4.0
3.0	6.0
2.0	6.0
3.0	8.0

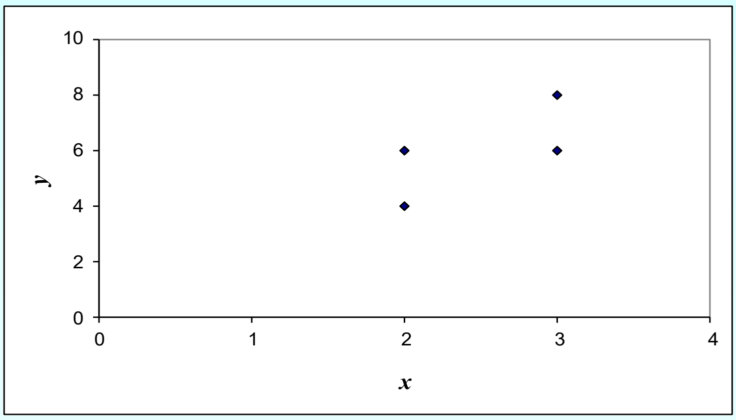


Figure. Data points for y vs x data.

Linear Regression-Criteria#1

Using $y=4x-4$ as the regression curve

Table. Residuals at each point for regression model $y=4x-4$

x	y	$y_{predicted}$	$E = y - y_{predicted}$
2.0	4.0	4.0	0.0
3.0	6.0	8.0	-2.0
2.0	6.0	4.0	2.0
3.0	8.0	8.0	0.0
			$\sum_{i=1}^{4} E_i = 0$

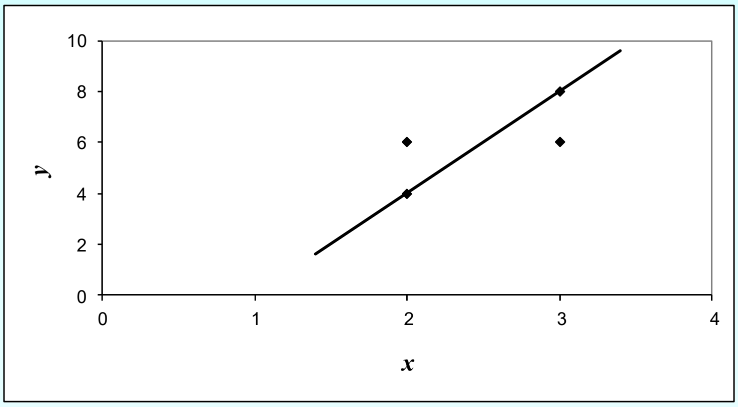


Figure. Regression curve $y=4x-4$ and y vs x data

Linear Regression-Criterion#1

Using $y=6$ as a regression curve

Table. Residuals at each point for regression model $y=6$

x	y	$y_{predicted}$	$E = y - y_{predicted}$
2.0	4.0	6.0	-2.0
3.0	6.0	6.0	0.0
2.0	6.0	6.0	0.0
3.0	8.0	6.0	2.0
			$\sum_{i=1}^{4} E_i = 0$

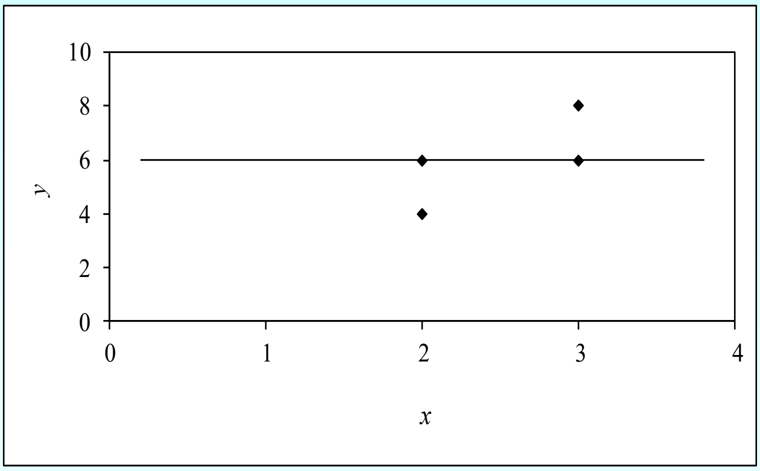


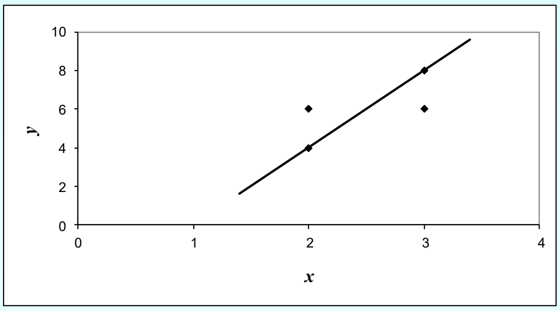
Figure. Regression curve $y=6$ and y vs x data

Linear Regression – Criterion #1

$\sum_{i=1}^{4} E_i = 0$ for both regression models of y=4x-4 and y=6

The sum of the residuals is minimized, in this case it is zero, but the regression model is not unique.

Hence the criterion of minimizing the sum of the residuals is a bad criterion.



Linear Regression-Criterion#2

Will minimizing $\sum_{i=1}^{n} |E_i|$ work any better?

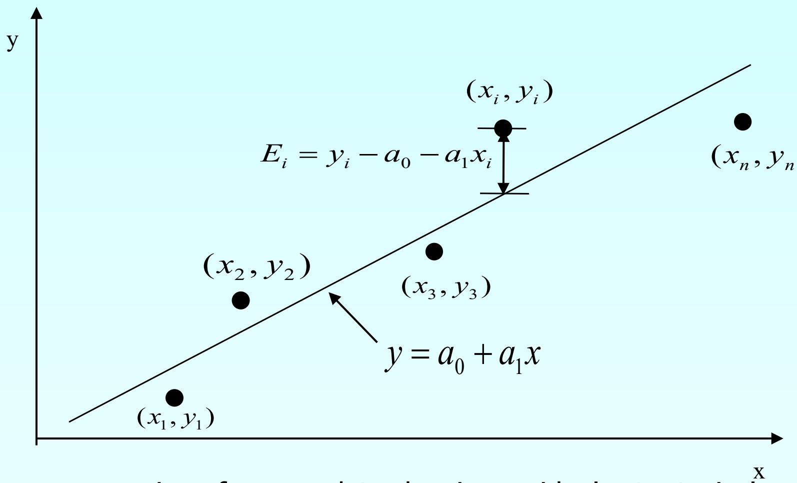


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i .

Example for Criterion#2

Example: Given the data points (2,4), (3,6), (2,6) and (3,8), best fit the data to a straight line using Criterion#2

Minimize $\sum_{i=1}^{n} |E_i|$

Table. Data Points

x	y
2.0	4.0
3.0	6.0
2.0	6.0
3.0	8.0

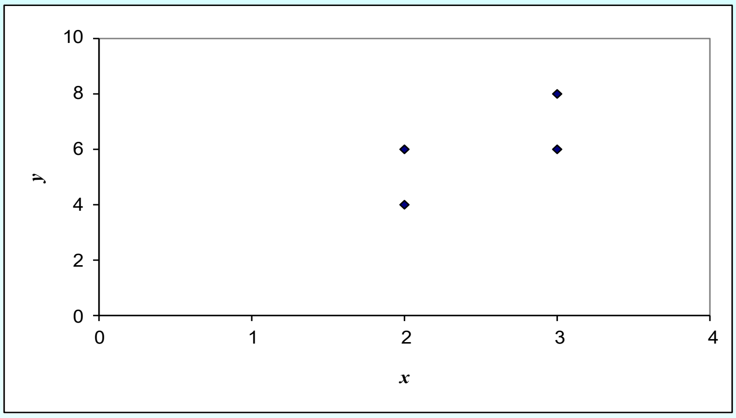


Figure. Data points for y vs. x data.

Linear Regression-Criterion#2

Using $y=4x-4$ as the regression curve

Table. Residuals at each point for regression model $y=4x-4$

x	y	$y_{predicted}$	$E = y - y_{predicted}$
2.0	4.0	4.0	0.0
3.0	6.0	8.0	-2.0
2.0	6.0	4.0	2.0
3.0	8.0	8.0	0.0
			$\sum_{i=1}^{4} \lvert E_i \rvert = 4$

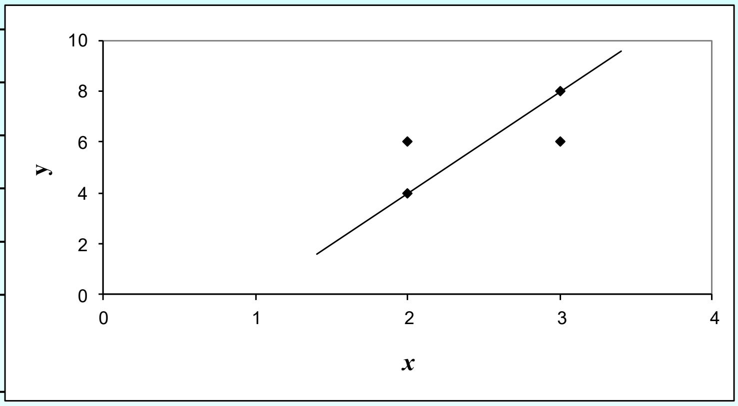


Figure. Regression curve $y= y=4x-4$ and y vs. x data

Linear Regression-Criterion#2

Using y=6 as a regression curve

Table. Residuals at each point for regression model y=6

x	y	$y_{predicted}$	$E = y - y_{predicted}$
2.0	4.0	6.0	-2.0
3.0	6.0	6.0	0.0
2.0	6.0	6.0	0.0
3.0	8.0	6.0	2.0
			$\sum_{i=1}^{4} \lvert E_i \rvert = 4$

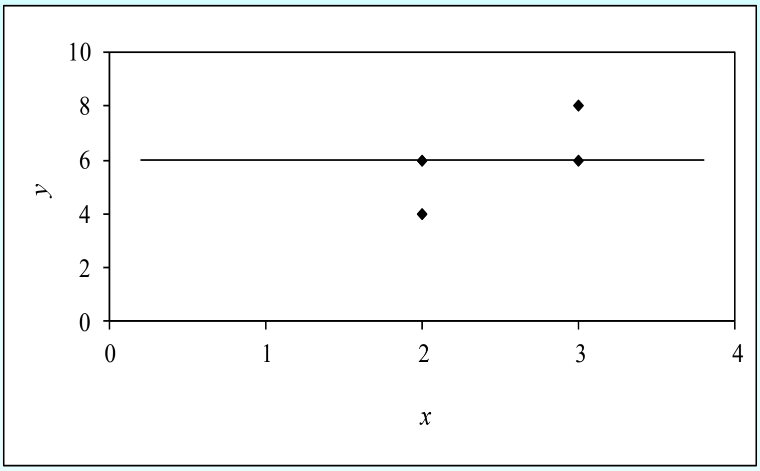


Figure. Regression curve y=6 and y vs x data

Linear Regression-Criterion#2

$\sum_{i=1}^{4} \lvert E_i \rvert = 4$ for both regression models of $y=4x-4$ and $y=6$.

The sum of the absolute residuals has been made as small as possible, that is 4, but the regression model is not unique.

Hence the criterion of minimizing the sum of the absolute value of the residuals is also a bad criterion.

Least Squares Criterion

The least squares criterion minimizes the sum of the square of the residuals in the model, and also produces a unique line.

$$S_r = \sum_{i=1}^{n} E_i^{\ 2} = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$$

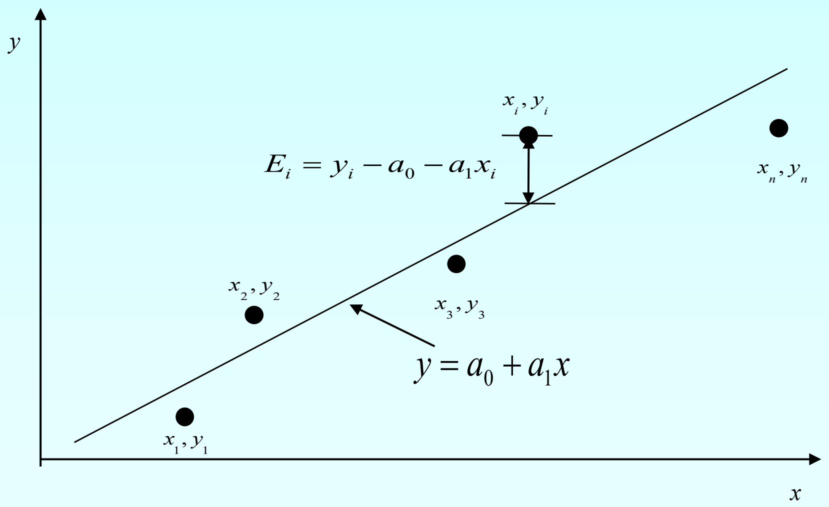


Figure. Linear regression of y vs x data showing residuals at a typical point, x_i.

Finding Constants of Linear Model

Minimize the sum of the square of the residuals: $S_r = \sum_{i=1}^{n} E_i^{\ 2} = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$

To find a_0 and a_1 we minimize S_r with respect to a_1 and a_0.

$$\frac{\partial S_r}{\partial a_0} = -2\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)(-x_i) = 0$$

giving

$$\sum_{i=1}^{n} a_0 + \sum_{i=1}^{n} a_1 x_i = \sum_{i=1}^{n} y_i$$

$$\sum_{i=1}^{n} a_0 x_i + \sum_{i=1}^{n} a_1 x_i^{\ 2} = \sum_{i=1}^{n} y_i x_i$$

Finding Constants of Linear Model

Solving for a_0 and a_1 directly yields,

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

and

$$a_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad a_0 = \bar{y} - a_1 \bar{x}$$

Example 1

The torque, T needed to turn the torsion spring of a mousetrap through an angle, is given below. Find the constants for the model given by $T = k_1 + k_2\theta$

Table: Torque vs Angle for a torsional spring

Angle, θ	Torque, T
Radians	*N-m*
0.698132	0.188224
0.959931	0.209138
1.134464	0.230052
1.570796	0.250965
1.919862	0.313707

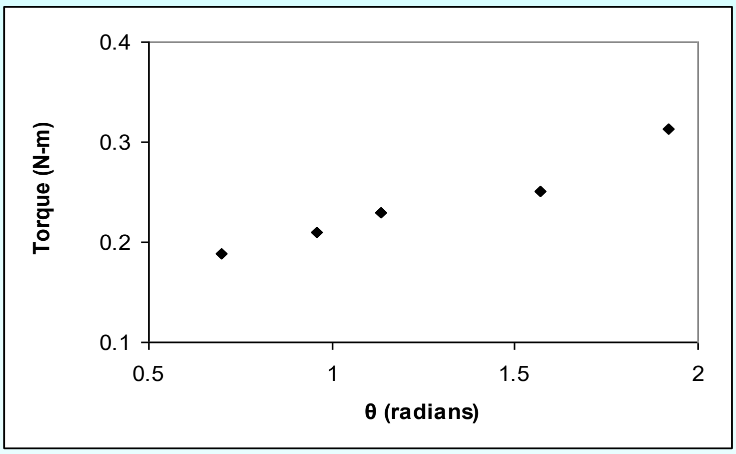


Figure. Data points for Torque vs Angle data

Example 1 cont.

The following table shows the summations needed for the calculations of the constants in the regression model.

Table. Tabulation of data for calculation of important summations

	θ	T	θ^2	$T\theta$
	Radians	*N-m*	*Radians²*	*N-m-Radians*
	0.698132	0.188224	0.487388	0.131405
	0.959931	0.209138	0.921468	0.200758
	1.134464	0.230052	1.2870	0.260986
	1.570796	0.250965	2.4674	0.394215
	1.919862	0.313707	3.6859	0.602274
$\sum_{i=1}^{5} =$	6.2831	1.1921	8.8491	1.5896

Using equations described for a_0 and a_1 with $n = 5$

$$k_2 = \frac{n\sum_{i=1}^{5}\theta_i T_i - \sum_{i=1}^{5}\theta_i \sum_{i=1}^{5} T_i}{n\sum_{i=1}^{5}\theta_i^2 - \left(\sum_{i=1}^{5}\theta_i\right)^2}$$

$$= \frac{5(1.5896) - (6.2831)(1.1921)}{5(8.8491) - (6.2831)^2}$$

$= 9.6091 \times 10^{-2}$ *N-m/rad*

Example 1 cont.

Use the average torque and average angle to calculate k_1

$$\bar{T} = \frac{\sum_{i=1}^{5} T_i}{n} = \frac{1.1921}{5} = 2.3842 \times 10^{-1}$$

$$\bar{\theta} = \frac{\sum_{i=1}^{5} \theta_i}{n} = \frac{6.2831}{5} = 1.2566$$

Using,

$$k_1 = \bar{T} - k_2\,\bar{\theta}$$

$$= 2.3842 \times 10^{-1} - (9.6091 \times 10^{-2})(1.2566)$$

$= 1.1767 \times 10^{-1}$ *N-m*

Example 1 Results

Using linear regression, a trend line is found from the data

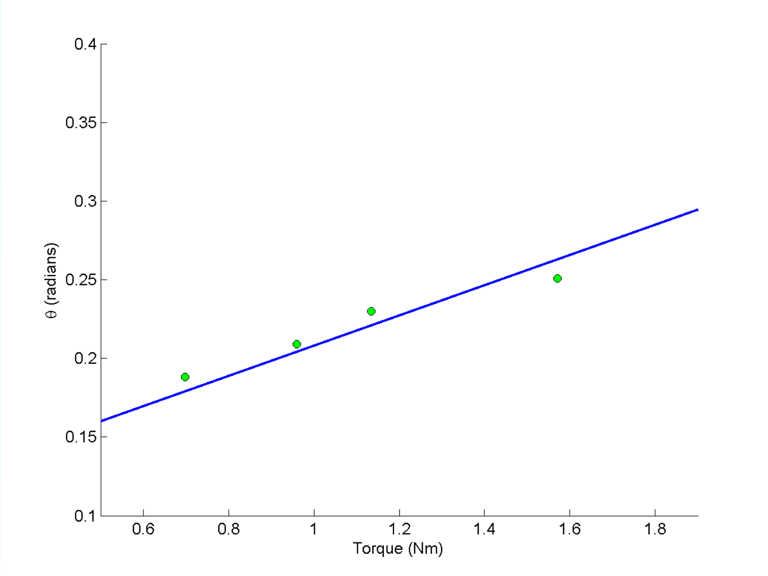


Figure. Linear regression of Torque versus Angle data

Can you find the energy in the spring if it is twisted from 0 to 180 degrees?

Linear Regression (special case)

Given

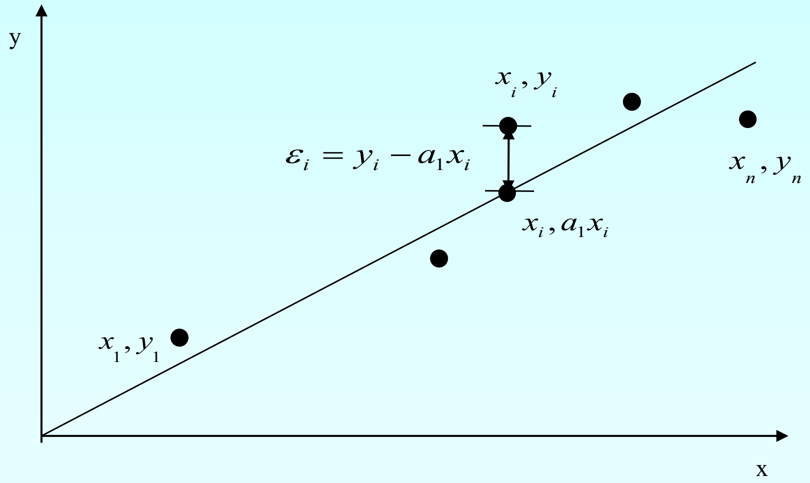
$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

best fit

$$y = a_1 x$$

to the data.

Linear Regression (special case cont.)



Linear Regression (special case cont.)

Residual at each data point

$$\varepsilon_i = y_i - a_1 x_i$$

Sum of square of residuals

$$S_r = \sum_{i=1}^{n} \varepsilon_i^{\ 2}$$

$$= \sum_{i=1}^{n} \left(y_i - a_1 x_i\right)^2$$

Linear Regression (special case cont.)

Differentiate with respect to a_1

$$\frac{dS_r}{da_1} = \sum_{i=1}^{n} 2(y_i - a_1 x_i)(-x_i)$$

$$= \sum_{i=1}^{n} \left(-2y_i x_i + 2a_1 x_i^{\ 2}\right)$$

$$\frac{dS_r}{da_1} = 0$$

gives

$$a_1 = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

Linear Regression (special case cont.)

Does this value of a_1 correspond to a local minima or local maxima?

$$a_1 = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

$$\frac{dS_r}{da_1} = \sum_{i=1}^{n} \left(-2y_i x_i + 2a_1 x_i^{\ 2}\right)$$

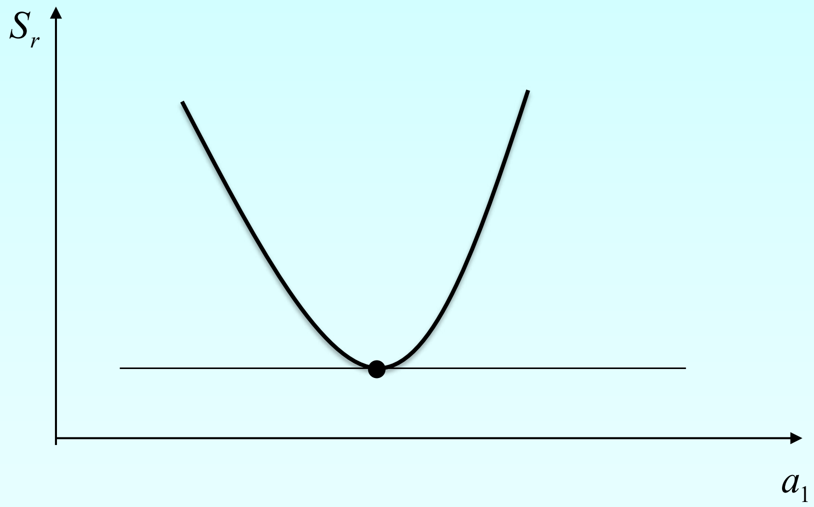
$$\frac{d^2 S_r}{da_1^{\ 2}} = \sum_{i=1}^{n} 2x_i^{\ 2} > 0$$

Yes, it corresponds to a local minima.

$$a_1 = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

Linear Regression (special case cont.)

S_r S_r



Example 2

To find the longitudinal modulus of composite, the following data is collected. Find the longitudinal modulus, E using the regression model $\sigma = E\varepsilon$ and the sum of the square of the residuals.

Table. Stress vs. Strain data

Strain	Stress
(%)	*(MPa)*
0	0
0.183	306
0.36	612
0.5324	917
0.702	1223
0.867	1529
1.0244	1835
1.1774	2140
1.329	2446
1.479	2752
1.5	2767
1.56	2896

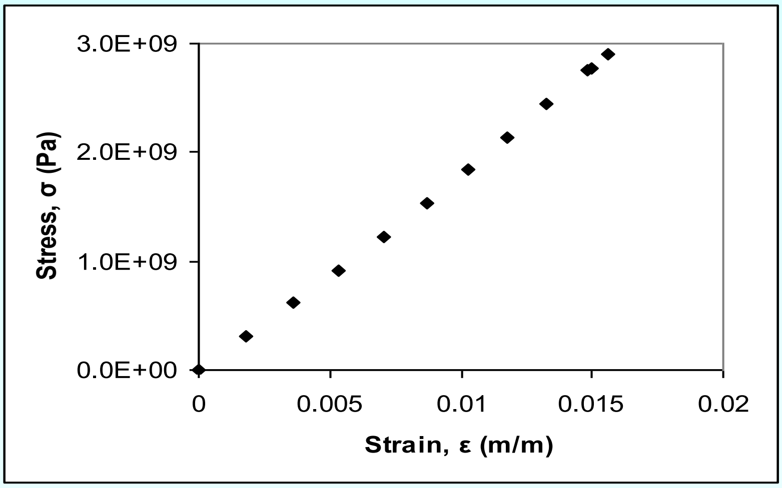


Figure. Data points for Stress vs. Strain data

Example 2 cont.

Table. Summation data for regression model

i	ε	σ	ε^2	εσ
1	0.0000	0.0000	0.0000	0.0000
2	1.8300×10^{-3}	3.0600×10^{8}	3.3489×10^{-6}	5.5998×10^{5}
3	3.6000×10^{-3}	6.1200×10^{8}	1.2960×10^{-5}	2.2032×10^{6}
4	5.3240×10^{-3}	9.1700×10^{8}	2.8345×10^{-5}	4.8821×10^{6}
5	7.0200×10^{-3}	1.2230×10^{9}	4.9280×10^{-5}	8.5855×10^{6}
6	8.6700×10^{-3}	1.5290×10^{9}	7.5169×10^{-5}	1.3256×10^{7}
7	1.0244×10^{-2}	1.8350×10^{9}	1.0494×10^{-4}	1.8798×10^{7}
8	1.1774×10^{-2}	2.1400×10^{9}	1.3863×10^{-4}	2.5196×10^{7}
9	1.3290×10^{-2}	2.4460×10^{9}	1.7662×10^{-4}	3.2507×10^{7}
10	1.4790×10^{-2}	2.7520×10^{9}	2.1874×10^{-4}	4.0702×10^{7}
11	1.5000×10^{-2}	2.7670×10^{9}	2.2500×10^{-4}	4.1505×10^{7}
12	1.5600×10^{-2}	2.8960×10^{9}	2.4336×10^{-4}	4.5178×10^{7}
$\sum_{i=1}^{12}$			1.2764×10^{-3}	2.3337×10^{8}

$$E=\frac{\sum_{i=1}^{n}\sigma_i\varepsilon_i}{\sum_{i=1}^{n}\varepsilon_i^{\ 2}}$$

$$\sum_{i=1}^{12}\varepsilon_i^2 = 1.2764\times10^{-3}$$

$$\sum_{i=1}^{12}\sigma_i\varepsilon_i = 2.3337\times10^{8}$$

$$E=\frac{\sum_{i=1}^{12}\sigma_i\varepsilon_i}{\sum_{i=1}^{12}\varepsilon_i^{\ 2}}$$

$$=\frac{2.3337\times10^{8}}{1.2764\times10^{-3}}$$

$$=182.84\ GPa$$

Example 2 Results

The equation $\sigma = 182.84\times10^{9}\,\varepsilon$ describes the data.

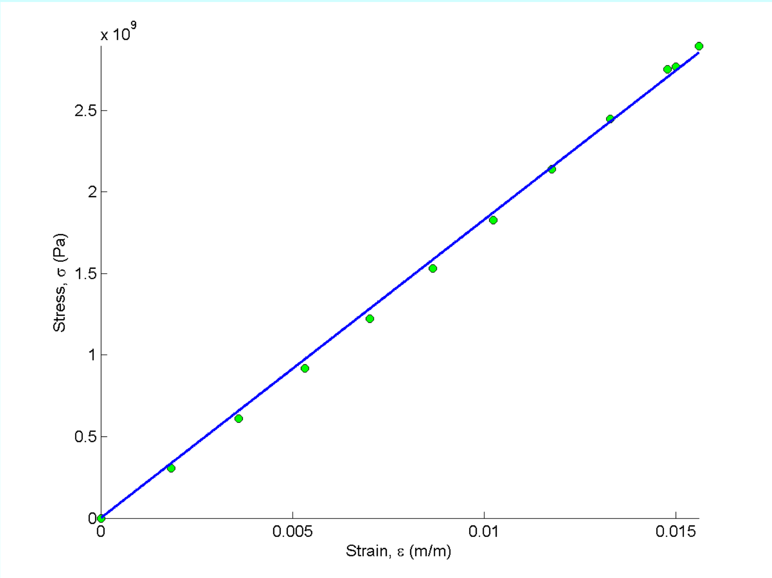


Figure. Linear regression for stress vs. strain data

THE END

Nonlinear Regression

Author: Autar Kaw et. al.

TEXTBOOK: NUMERICAL METHODS WITH APPLICATIONS

Nonlinear Regression

Nonlinear Regression

Some popular nonlinear regression models:

1. Exponential model: $(y = ae^{bx})$
2. Polynomial model: $(y = a_0 + a_1 x + \ldots + a_m x^m)$
3. Saturation growth model: $\left(y = \dfrac{ax}{b+x}\right)$
4. Power model: $(y = ax^b)$

Nonlinear Regression

Given n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = f(x)$ to the data, where $f(x)$ is a nonlinear function of x .

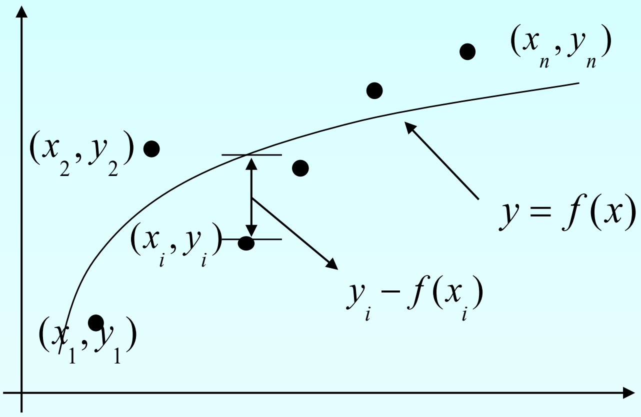


Figure. Nonlinear regression model for discrete y vs. x data

Regression
Exponential Model

Exponential Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = ae^{bx}$ to the data.

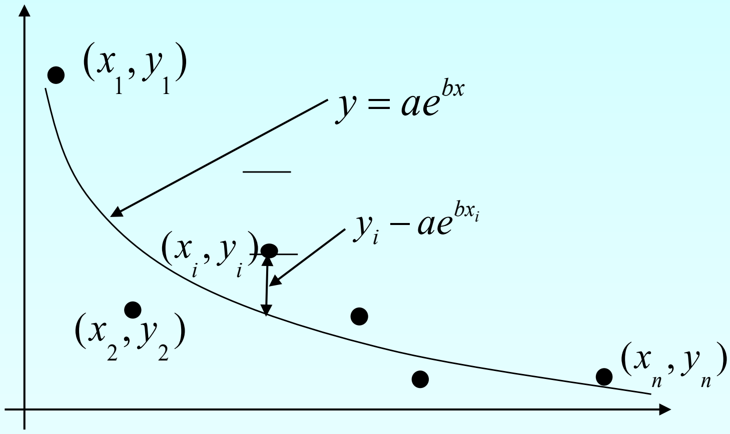


Figure. Exponential model of nonlinear regression for y vs. x data

Finding Constants of Exponential Model

The sum of the square of the residuals is defined as

$$S_r = \sum_{i=1}^{n} \left(y_i - ae^{bx_i} \right)^2$$

Differentiate with respect to *a* and *b*

$$\frac{\partial S_r}{\partial a} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i} \right)\left(-e^{bx_i} \right) = 0$$

$$\frac{\partial S_r}{\partial b} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i} \right)\left(-ax_i e^{bx_i} \right) = 0$$

Finding Constants of Exponential Model

Rewriting the equations, we obtain

$$-\sum_{i=1}^{n} y_i e^{bx_i} + a\sum_{i=1}^{n} e^{2bx_i} = 0$$

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - a\sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

Finding constants of Exponential Model

Solving the first equation for a yields

$$a = \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}}$$

Substituting a back into the previous equation

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

The constant b can be found through numerical methods such as bisection method.

Example 1-Exponential Model

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the Technetium-99m would be gone in about 6 hours. It, however, takes about 24 hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

Table. Relative intensity of radiation as a function of time.

t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

Example 1-Exponential Model cont.

The relative intensity is related to time by the equation

$$\gamma = Ae^{\lambda t}$$

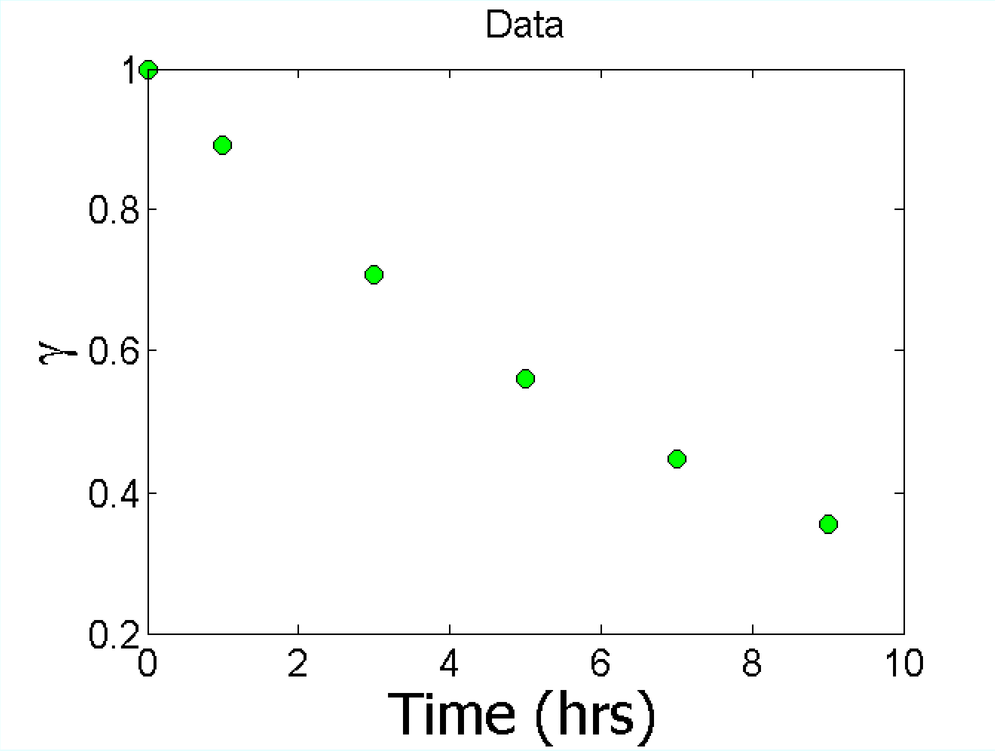
Find:

a) The value of the regression constants A and λ

b) The half-life of Technetium-99m

c) Radiation intensity after 24 hours

Plot of data



Constants of the Model

$$\gamma = Ae^{\lambda t}$$

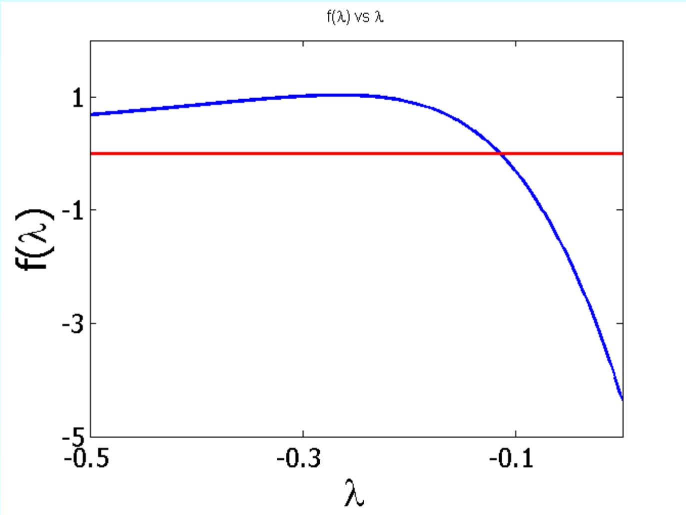
The value of λ is found by solving the nonlinear equation

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$

$$A = \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}}$$

Setting up the Equation in Python

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$



t (hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

Setting up the Equation in Python

$$f(\lambda) = \sum_{i=1}^{n} \gamma_i t_i e^{\lambda t_i} - \frac{\sum_{i=1}^{n} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{n} e^{2\lambda t_i}} \sum_{i=1}^{n} t_i e^{2\lambda t_i} = 0$$

$$\lambda = -0.1151$$

```
t=[0 1  3  5  7  9]
gamma=[1  0.891  0.708  0.562  0.447  0.355]
syms lamda
sum1=sum(gamma.*t.*exp(lamda*t));
sum2=sum(gamma.*exp(lamda*t));
sum3=sum(exp(2*lamda*t));
sum4=sum(t.*exp(2*lamda*t));
f=sum1-sum2/sum3*sum4;
```

Calculating the Other Constant

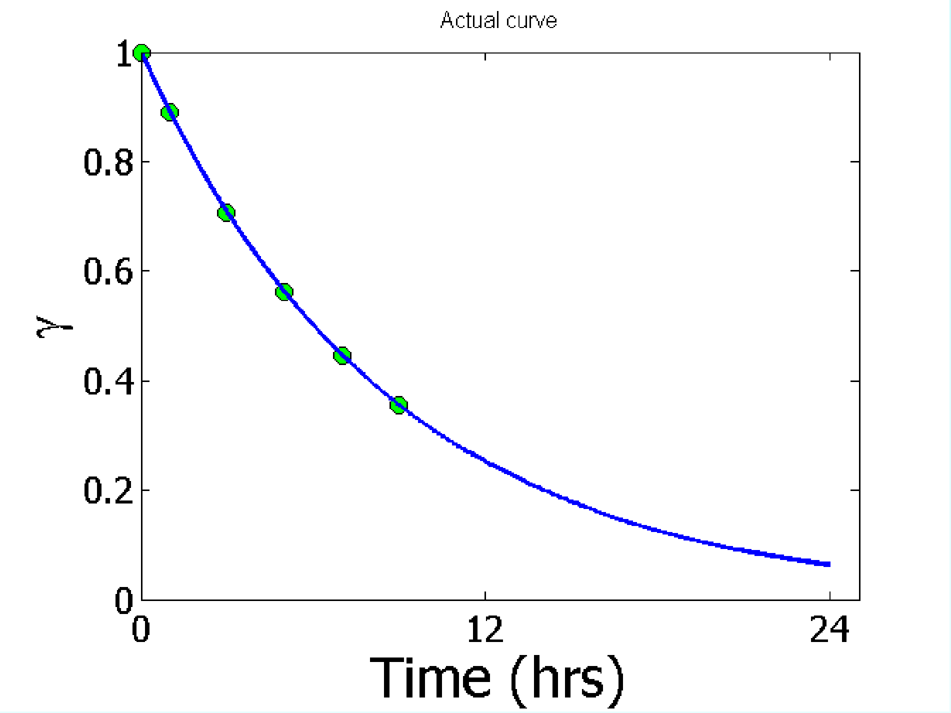
The value of *A* can now be calculated

$$A = \frac{\sum_{i=1}^{6} \gamma_i e^{\lambda t_i}}{\sum_{i=1}^{6} e^{2\lambda t_i}} = 0.9998$$

The exponential regression model then is

$$\gamma = 0.9998\ e^{-0.1151t}$$

Plot of data and regression curve



Relative Intensity After 24 hrs

The relative intensity of radiation after 24 hours

$$\gamma = 0.9998 \times e^{-0.1151(24)}$$

$$= 6.3160 \times 10^{-2}$$

This result implies that only

$$\frac{6.316 \times 10^{-2}}{0.9998} \times 100 = 6.317\%$$

radioactive intensity is left after 24 hours.

Homework

- What is the half-life of Technetium-99m isotope?
- Write a program in the language of your choice to find the constants of the model.
- Compare the constants of this regression model with the one where the data is transformed.
- What if the model was $\gamma = e^{\lambda t}$?

Polynomial Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = a_0 + a_1 x + \ldots + a_m x^m$ $(m \leq n-2)$ to a given data set.

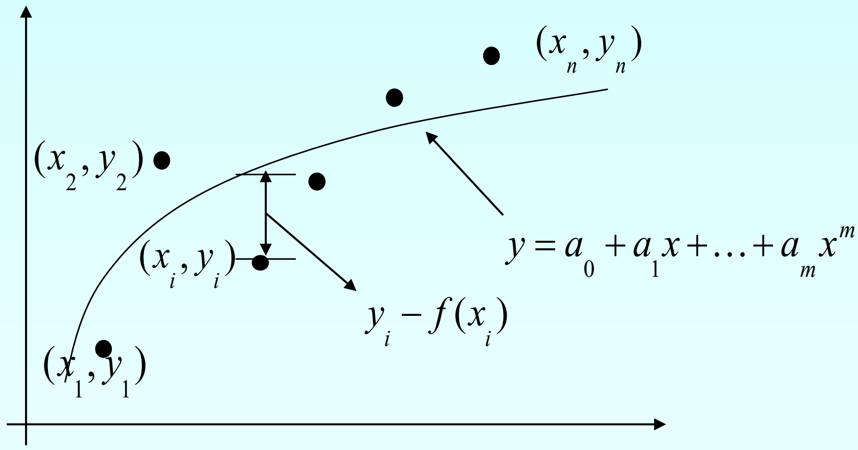


Figure. Polynomial model for nonlinear regression of y vs. x data

Polynomial Model cont.

The residual at each data point is given by

$$E_i = y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m$$

The sum of the square of the residuals then is

$$S_r = \sum_{i=1}^{n} E_i^2$$

$$= \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m \right)^2$$

Polynomial Model cont.

To find the constants of the polynomial model, we set the derivatives with respect to a_i where $i = 1,\ldots m,$ equal to zero.

$$\frac{\partial S_r}{\partial a_0} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \; . \; . - a_m x_i^m\right)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \; . \; . - a_m x_i^m\right)(-x_i) = 0$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$\frac{\partial S_r}{\partial a_m} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - . \; . \; . - a_m x_i^m\right)(-x_i^m) = 0$$

Polynomial Model cont.

These equations in matrix form are given by

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} x_i\right) & . \; . \; . & \left(\sum_{i=1}^{n} x_i^m\right) \\ \left(\sum_{i=1}^{n} x_i\right) & \left(\sum_{i=1}^{n} x_i^2\right) & . \; . \; . & \left(\sum_{i=1}^{n} x_i^{m+1}\right) \\ . \; . \; . & . \; . \; . & . \; . \; . & . \; . \; . \\ \left(\sum_{i=1}^{n} x_i^m\right) & \left(\sum_{i=1}^{n} x_i^{m+1}\right) & . \; . \; . & \left(\sum_{i=1}^{n} x_i^{2m}\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ . \; . \; . \\ a_m \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ . \; . \; . \\ \sum_{i=1}^{n} x_i^m y_i \end{bmatrix}$$

The above equations are then solved for $a_0, a_1, \ldots, a_m$

Example 2-Polynomial Model

Regress the thermal expansion coefficient vs. temperature data to a second order polynomial.

Table. Data points for temperature vs α

Temperature, T (°F)	Coefficient of thermal expansion, α (in/in/°F)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

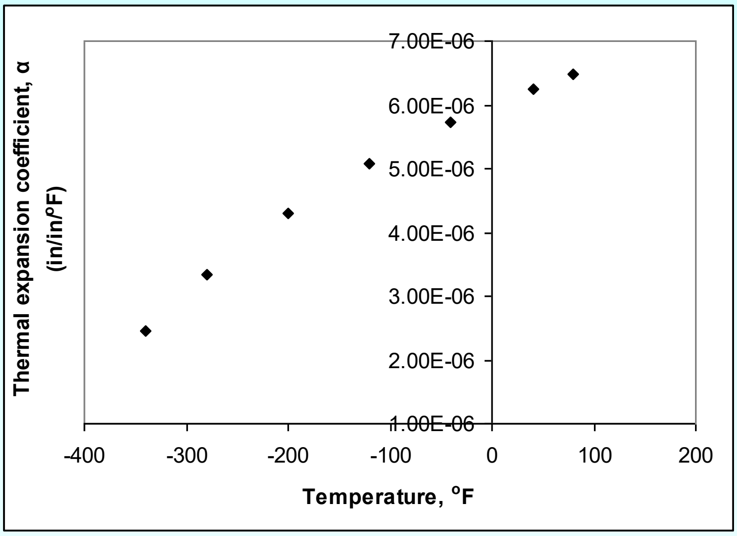


Figure. Data points for thermal expansion coefficient vs temperature.

Example 2-Polynomial Model cont.

We are to fit the data to the polynomial regression model

$$\alpha = a_0 + a_1 T + a_2 T^2$$

The coefficients a_0, a_1, a_2 are found by differentiating the sum of the square of the residuals with respect to each variable and setting the values equal to zero to obtain

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) \\ \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) \\ \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) & \left(\sum_{i=1}^{n} T_i^4\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} \alpha_i \\ \sum_{i=1}^{n} T_i\,\alpha_i \\ \sum_{i=1}^{n} T_i^2 \alpha_i \end{bmatrix}$$

Example 2-Polynomial Model cont.

The necessary summations are as follows

Table. Data points for temperature vs. α

Temperature, T (ºF)	Coefficient of thermal expansion, α (in/in/ºF)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

$$\sum_{i=1}^{7} T_i^2 = 2.5580\times10^{5}$$

$$\sum_{i=1}^{7} T_i^3 = -7.0472\times10^{7}$$

$$\sum_{i=1}^{7} T_i^4 = 2.1363\times10^{10}$$

$$\sum_{i=1}^{7} \alpha_i = 3.3600\times10^{-5}$$

$$\sum_{i=1}^{7} T_i\alpha_i = -2.6978\times10^{-3}$$

$$\sum_{i=1}^{7} T_i^2\alpha_i = 8.5013\times10^{-1}$$

Example 2-Polynomial Model cont.

Using these summations, we can now calculate a_0, a_1, a_2

$$\begin{bmatrix} 7.0000 & -8.6000\times10^{2} & 2.5800\times10^{5} \\ -8.600\times10^{2} & 2.5800\times10^{5} & -7.0472\times10^{7} \\ 2.5800\times10^{5} & -7.0472\times10^{7} & 2.1363\times10^{10} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 3.3600\times10^{-5} \\ -2.6978\times10^{-3} \\ 8.5013\times10^{-1} \end{bmatrix}$$

Solving the above system of simultaneous linear equations we have

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 6.0217\times10^{-6} \\ 6.2782\times10^{-9} \\ -1.2218\times10^{-11} \end{bmatrix}$$

The polynomial regression model is then

$$\alpha = a_0 + a_1 T + a_2 T^2$$
$$= 6.0217\times10^{-6} + 6.2782\times10^{-9}\,\mathrm{T} - 1.2218\times10^{-11}\,\mathrm{T}^2$$

Transformation of Data

To find the constants of many nonlinear models, it results in solving simultaneous nonlinear equations. For mathematical convenience, some of the data for such models can be transformed. For example, the data for an exponential model can be transformed.

As shown in the previous example, many chemical and physical processes are governed by the equation,

$$y = ae^{bx}$$

Taking the natural log of both sides yields,

$$\ln y = \ln a + bx$$

Let $z = \ln y$ and $a_0 = \ln a$

We now have a linear regression model where $z = a_0 + a_1 x$

(implying) $a = e^{a_o}$ with $a_1 = b$

Transformation of data cont.

Using linear model regression methods,

$$a_1 = \frac{n\sum_{i=1}^{n} x_i z_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$a_0 = \bar{z} - a_1 \bar{x}$$

Once a_o, a_1 are found, the original constants of the model are found as

$$b = a_1$$

$$a = e^{a_0}$$

Example 3-Transformation of data

Many patients get concerned when a test involves injection of a radioactive material. For example for scanning a gallbladder, a few drops of Technetium-99m isotope is used. Half of the Technetium-99m would be gone in about 6 hours. It, however, takes about 24 hours for the radiation levels to reach what we are exposed to in day-to-day activities. Below is given the relative intensity of radiation as a function of time.

Table. Relative intensity of radiation as a function of time

t(hrs)	0	1	3	5	7	9
γ	1.000	0.891	0.708	0.562	0.447	0.355

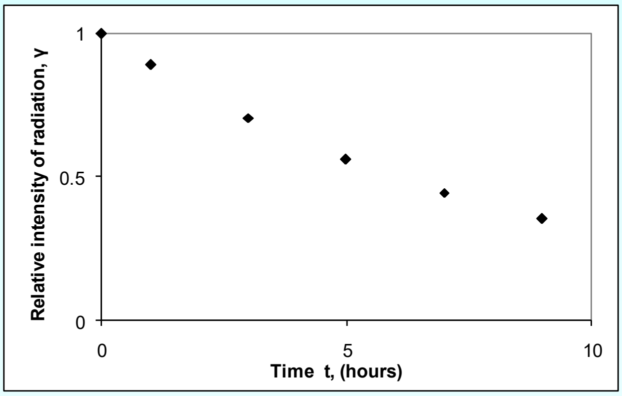


Figure. Data points of relative radiation intensity vs. time

Example 3-Transformation of data cont.

Find:

a) The value of the regression constants A and λ

b) The half-life of Technetium-99m

c) Radiation intensity after 24 hours

The relative intensity is related to time by the equation

$$\gamma = Ae^{\lambda t}$$

Example 3-Transformation of data cont.

Exponential model given as,

$$\gamma = Ae^{\lambda t}$$

$$\ln(\gamma) = \ln(A) + \lambda t$$

Assuming $z = \ln \gamma$, $a_o = \ln(A)$ and $a_1 = \lambda$ we obtain

$$z = a_0 + a_1 t$$

This is a linear relationship between z and t

Example 3-Transformation of data cont.

Using this linear relationship, we can calculate a_0, a_1 where

$$a_1 = \frac{n\sum_{i=1}^{n} t_i z_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} t_1^2 - \left(\sum_{i=1}^{n} t_i\right)^2}$$

and

$$a_0 = \bar{z} - a_1 \bar{t}$$

$$\lambda = a_1$$

$$A = e^{a_0}$$

Example 3-Transformation of Data cont.

Summations for data transformation are as follows

Table. Summation data for Transformation of data model

i	t_i	γ_i	$z_i = \ln \gamma_i$	$t_i z_i$	t_i^2
1	0	1	0.00000	0.0000	0.0000
2	1	0.891	−0.11541	−0.11541	1.0000
3	3	0.708	−0.34531	−1.0359	9.0000
4	5	0.562	−0.57625	−2.8813	25.000
5	7	0.447	−0.80520	−5.6364	49.000
6	9	0.355	−1.0356	−9.3207	81.000
$\sum$	25.000		−2.8778	−18.990	165.00

With $n = 6$

$$\sum_{i=1}^{6} t_i = 25.000$$

$$\sum_{i=1}^{6} z_i = -2.8778$$

$$\sum_{i=1}^{6} t_i z_i = -18.990$$

$$\sum_{i=1}^{6} t_i^2 = 165.00$$

Example 3-Transformation of Data cont.

Calculating a_0, a_1

$$a_1 = \frac{6(-18.990) - (25)(-2.8778)}{6(165.00) - (25)^2} = -0.11505$$

$$a_0 = \frac{-2.8778}{6} - (-0.11505)\frac{25}{6} = -2.6150 \times 10^{-4}$$

Since

$$a_0 = \ln(A)$$

$$A = e^{a_0}$$

$$= e^{-2.6150 \times 10^{-4}} = 0.99974$$

also

$$\lambda = a_1 = -0.11505$$

Example 3-Transformation of Data cont.

Resulting model is $\gamma = 0.99974 \times e^{-0.11505t}$

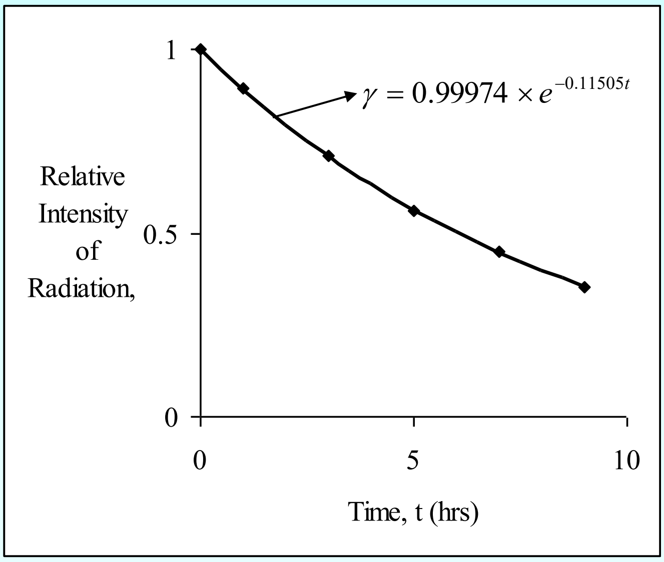


Figure. Relative intensity of radiation as a function of temperature using transformation of data model.

Example 3-Transformation of Data cont.

The regression formula is then

$$\gamma = 0.99974 \times e^{-0.11505t}$$

b) Half life of Technetium-99m is when $\gamma = \frac{1}{2}\gamma\Big|_{t=0}$

$$0.99974 \times e^{-0.11505t} = \frac{1}{2}(0.99974)e^{-0.11505(0)}$$

$$e^{-0.11508t} = 0.5$$

$$-0.11505t = \ln(0.5)$$

$$t = 6.0248 \ hours$$

Example 3-Transformation of Data cont.

c) The relative intensity of radiation after 24 hours is then

$$\gamma = 0.99974\,e^{-0.11505(24)}$$
$$= 0.063200$$

This implies that only $\dfrac{6.3200\times10^{-2}}{0.99983}\times100 = 6.3216\%$ of the radiative material is left after 24 hours.

Comparison

Comparison of exponential model with and without data Transformation:

Table. Comparison for exponential model with and without data Transformation.

	With data Transformation (Example 3)	Without data Transformation (Example 1)
A	0.99974	0.99983
λ	−0.11505	−0.11508
Half-Life (hrs)	6.0248	6.0232
Relative intensity after 24 hrs.	6.3200×10^{-2}	6.3160×10^{-2}

THE END