Roots of Equations

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Numerical Analysis of Engineering Systems

February 10, 2014

Outline

- Review last lecture
- Continue numerical solution of algebraic equations
- Desired accuracy in iterations
- Methods for roots of equations
  - Bisection
  - Secant method
  - Newton's Method
  - False position (*regula falsi*)
  - Successive substitution

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Review Computing

- Representation of numbers to any base
- Use of binary storage in computers
- For integer numbers the bit size of the storage limits the range (VBA integer from –32,768 to 32,767 and long from –2,147,483,648$_{10}$ to 2,147,483,647
- For real numbers storage size affects significant figures and magnitude
  - Single 1.4x10^{-45} to 3.4x10^{38} (~7 sig figs)
  - Double 4.9x10^{-324} to 1.8x10^{308} (~15 sig figs)

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Review Solution of Equations

- Want solution to equations like ax = sin(x) for a given value of a
- It is one equation in one unknown, but we cannot get an explicit solution of the form x = calculated result
  - It is also possible that there will be more than one solution to the equation
  - Root is another word for solution
- Can look at solution graphically (like a graphing calculator)

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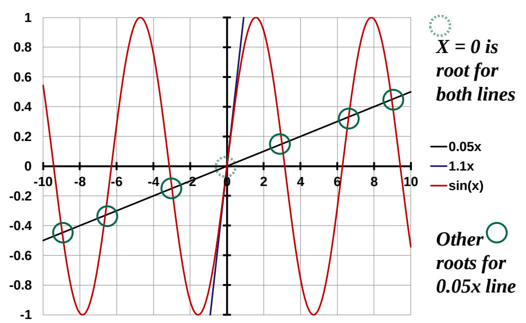
Review Plot of Roots



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Review Finding Roots

- Can write all equations as f(x) = 0
  - Simply move all terms to left-hand side
- Use trial and error algorithms
  - Two classes of methods
    - One initial guess
    - Two initial guesses that "bracket" root (*i.e.* root lies between the initial guesses)
  - Methods that bracket root are usually slower but surer
  - May need separate iteration process to get initial guesses bracketing root

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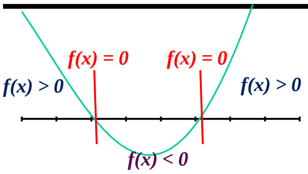
Review Bracketing a Root



Plot shows two roots, f(x) = 0 and values of f(x) on opposite sides of root

- Basic idea: when a root, f(x) = 0, is bracketed the values of f(x) on opposite sides of the root have opposite signs
- If $f(x)f(x+\Delta x) < 0$ there is a root, f(x) = 0, between x and $x+\Delta x$

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Review Process and Notation

- Iteration process has one or more initial guesses, called x_0, x_1 , etc. of root
  - Usually have one or two initial guesses
- Iteration procedure that uses previous estimates, x_k, x_{k-1}, etc. to find a new value x_{k+1}
  - In most cases two previous iterations are used, but some methods use one
- Iterations continues until x value is found that gives desired accuracy

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Review Process and Notation II

- Some algorithms maintain two current estimates that bracket a root
- The notation for these estimates is x_+ and x_- where $f(x_+) > 0$ and $f(x_-) < 0$
- In these algorithms the iteration computes a value of x_{new} from x_+ and x_-
- The value of x_{new} for iteration k is used as the iteration value x_{k+1} in error calculations on next slide

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What is Desired Accuracy

Note use of absolute values

- Three measures:
  - Small value of f: $|f| < \varepsilon_1$
  - Small value of change in x between iterations: $|x_{k+1} – x_k| < \varepsilon_2$
  - Small value of **relative** change in x between iterations: $|x_{k+1} – x_k| < \varepsilon_3|x_{k+1}|$
  - Can use combinations of the three approaches as “or” tests
  - Third approach, relative change in x, is often most useful since the goal is to find an accurate value of x

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Desired Accuracy in Code

- Typically use relative error in x
  - Converged is Boolean variable (true/false)
  - May also use condition directly in If statement

```
Converged = Abs(xk+1 – xk) ≤ _
desiredRelativeError * Abs(xk+1)
```

- Can also use dual test

```
Converged = Abs(f(xk+1)) ≤ _
              desiredErrorInF And _
                   Abs(xk+1 – xk) ≤ _
    desiredRelativeError * Abs(xk+1)
```

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Termination Condition

- What if you never get desired accuracy in iterations?
- Need to limit number of iterations
- If maximum iterations are exceeded return an error message
- Message may contain latest estimate and its relative error
- Will show coding examples later

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Review Secant Method

- Starts with two initial guesses, x_0 and x_1, which need not bracket root
- Each iteration uses values of two successive guesses, x_k and x_{k-1} to find new guess, x_{k+1}
- Approximate behavior of f(x) near guess as straight line gives algorithm

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

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Review Secant Example

- Solve f(x) = 0.05x – sin(x) = 0
- Pick x_0 = 2 and x_1 = 2.5
  - $f(x_0)$ = f(2) = 0.05(2) – sin(2) = –0.809
  - $f(x_1)$ = f(3) = 0.05(2.5) – sin(2.5) = –0.473

Initial guesses do not have to bracket root

- Apply general equation to first iteration

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

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

$$x_2 = 2.5 - (-0.473)\frac{2.5 - 2}{-0.473 - (-0.809)} = 3.20$$

$$f(x_2) = 0.05(3.20) - sin(3.21) = 0.224$$

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Review Secant Example II

- Note: All significant figures of calculator or spreadsheet used in calculations
  - Rounding shown here to save space
- Apply general equation to second iteration

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)}$$

$$x_3 = 3.20 - (0.224)\frac{3.20 - 2.5}{0.224 - (-0.473)} = 2.98$$

$$f(x_3) = 0.05(2.98) - sin(2.98) = -0.0131$$

Can you find x4 and $f(x_4)$?

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Review Secant Example III

k	x_k	$f(x_k)$	$\lvert x_k - x_{k-1}\rvert$
0	2	-8.09E-01	
1	2.5	-4.73E-01	5.0E-01
2	3.20493820516827	2.24E-01	7.0E-01
3	2.97884928100731	-1.31E-02	2.3E-01
4	2.99134973893018	-1.11E-04	1.3E-02
5	2.99145653304953	1.04E-07	1.1E-04
6	2.99145643339981	-7.95E-13	1.0E-07
7	2.99145643340058	0.00E+00	7.7E-13
8	2.99145643340058	0.00E+00	0.0E+00

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Review Secant Method Evaluation

- Simple method to use
- Generally converges to solution relatively quickly
- Iteration calculations not complex
- May not converge for certain problems
- Bad initial guesses may give incorrect root when equation has multiple roots

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Secant Method Exercise

- Find root of $f(x) = 3xe^{-x^2} - 1 = 0$
  - Start with initial guesses x_0 = 0 and x_1 = 1
  - Repeat the following steps to get a new guess, x_{k+1}, from the guesses x_k and x_{k-1}
  - Compute x_{k+1} from the equation

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

  - Compute $f(x_{k+1})$
- Repeat the process $|x_{k+1} - x_k| < 0.003\,|x_{k+1}|$

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Precedence Warning

- What is $-x^2$?
- Depends on the rules of precedence
- In VBA this is the same as $-(x^2)$
  - Exponentiation has higher precedence than unary minus
- On Excel worksheet this is the same as $(-x)^2$
  - Unary minus has higher precedence than exponentiation

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Solution to Secant Exercise

$$f(x_0) = 3x_0 e^{-x_0^2} - 1 = 3(0)e^{-0^2} - 1 = -1$$

$$f(x_1) = 3x_1 e^{-x_1^2} - 1 = 3(1)e^{-1^2} - 1 = 0.1036$$

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

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

$$x_2 = 1 - 0.1036\frac{1 - 0}{0.1036 - (-1)} = 0.9061$$

$|x_2 - x_1| = |0.9061 - 1| = 0.939 > 0.003\ |x_2| = 0.0027$

Not converged!

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Solution to Secant Exercise II

$$x_1 = 1 \quad f(x_1) = 0.1036$$

$$f(x_2) = 3x_2 e^{-x_2^2} - 1 = 3(0.9061)e^{-0.9061^2} - 1 = 0.1960$$

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)}$$

$$x_3 = 0.9061 - 0.1960\frac{0.9061 - 1}{0.1960 - 0.1036} = 1.105$$

$|x_3 - x_2| = |1.105 - 0.906| = 0.199 > 0.003\ |x_3| = 0.0033$

Not converged!

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Solution to Secant Exercise III

$$x_2 = 0.9061 \quad f(x_2) = 0.1960$$

$$f(x_3) = 3x_3 e^{-x_3^2} - 1 = 3(1.105)e^{-1.105^2} - 1 = -0.0228$$

$$x_4 = x_3 - f(x_3)\frac{x_3 - x_2}{f(x_3) - f(x_2)}$$

$$x_4 = 1.105 - (-0.0228)\frac{1.105 - 0.9061}{(-0.0228) - 0.1960} = 1.085$$

$|x_4 - x_3| = |1.085 - 1.105| = 0.021 > 0.003\ |x_4| = 0.0032$

Not converged!

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Solution to Secant Exercise IV

$$x_3 = 1.105 \quad f(x_3) = -0.0228$$

$$f(x_4) = 3x_4 e^{-x_4^2} - 1 = 3(1.085)e^{-1.085^2} - 1 = 3.449x10^{-3}$$

$$x_5 = x_4 - f(x_4)\frac{x_4 - x_3}{f(x_4) - f(x_3)}$$

$$x_5 = 1.085 - (3.449x10^{-3})\frac{1.085 - 1.105}{3.449x10^{-3} - (-0.0228)} = 1.087$$

$|x_5 - x_4| = |1.087 - 1.085| = 0.002 < 0.003\ |x_5| = 0.0033$

Converged!

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Solution to Secant Exercise V

k	x_k	$f(x_k)$	$x_k - x_{k-1}$
0	0	-1	
1	1	0.103638	1
2	0.9060939428197	0.196013	-0.093910
3	1.1053561023637	-0.022770	0.199262
4	1.0846185436620	0.003449	-0.020740
5	1.0873467119195	2.99E-05	0.002728
6	1.0873705979212	-4.20E-08	2.39E-05
7	1.0873705643998	5.08E-13	-3.40E-08
8	1.0873705644002	0	4.05E-13
9	1.0873705644002	0	0

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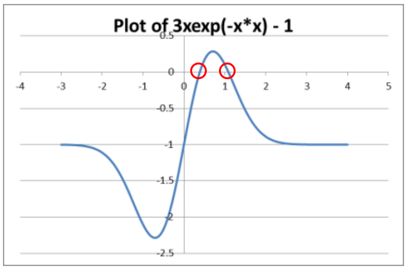
Secant Exercise Plot



Found one of two possible roots with initial guesses of 0 and 1; start with different initial guess for second root

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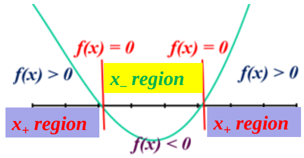
Root Bracketing



Plot shows two roots, f(x) = 0 and values of f(x) on opposite sides of root

- Basic idea: when a root, f(x) = 0, is bracketed the values of f(x) on opposite sides of the root have opposite signs
  - For bracketed root, define x_+ as value of x such that $f(x_+) > 0$ and x_- for $f(x_-) < 0$

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Bisection Method

- Start with two guesses x_+ and x_- that bracket a root with $f(x_+) > 0$ and $f(x_-) < 0$
- Repeat the following steps for the two current guesses x_+ and x_-
  - Compute the midpoint $x_{new} = (x_+ + x_-)/2$
  - If $f(x_{new}) > 0$ replace x_+ by x_{new}
  - Else replace x_- by x_{new}
- Continue this process until a value of x_{new} gives desired accuracy

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Bisection Method Example

- Find root of f(x) = 0.05x – sin(x) between x = 2 and x = 4
  - f(2) = 0.05(2) – sin(2) = –0.8093, so x_- = 2
  - f(4) = 0.05(4) – sin(4) = 0.9568, so x_+ = 4
  - Iteration 1: $x_{new} = (x_- + x_+)/2 = (2 + 4)/2 = 3$
    - $f(x_{new})$ = f(3) = 0.05(3) – sin(3) = 0.0088 >0
    - Set x_+ = 3 and leave x_- = 2
  - Iteratn 2: $x_{new} = (x_- + x_+)/2 = (2 + 3)/2 = 2.5$
    - $f(x_{new})$ = f(2.5) = 0.05(2.5) – sin(2.5) = -0.4735
    - Set x_- = 2.5 and leave x_+ = 3 because $f(x_{new})$<0

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Bisection Iterations

count	x_+	x_-	$f(x_+)$	$f(x_-)$	x_{new}	$f(x_{new})$
1	4	2	0.95680	-0.8093	3	0.00888
2	3	2	0.00888	-0.8093	2.5	-0.47347
3	3	2.5	0.00888	-0.47347	2.75	-0.24416
4	3	2.75	0.00888	-0.24416	2.875	-0.1197
5	3	2.875	0.00888	-0.1197	2.9375	-0.0558
6	3	2.9375	0.00888	-0.0558	2.96875	-0.02355
7	3	2.96875	0.00888	-0.02355	2.98438	-0.00735
8	3	2.98438	0.00888	-0.00735	2.99219	0.00076
9	2.99219	2.98438	0.00076	-0.00735	2.98828	-0.0033
10	2.99219	2.98828	0.00076	-0.0033	2.99023	-0.00127
11	2.99219	2.99023	0.00076	-0.00127	2.99121	-0.00026
12	2.99219	2.99121	0.00076	-0.00026	2.99170	0.00025
13	2.99170	2.99121	0.00025	-0.00026	2.99146	-1.4E-06
14	2.99170	2.99146	0.00025	-1.4E-06	2.99158	0.00013
15	2.99158	2.99146	0.00013	-1.4E-06	2.99152	6.2E-05
16	2.99152	2.99146	6.2E-05	-1.4E-06	2.99149	3.03E-05
17	2.99149	2.99146	3.03E-05	-1.4E-06	2.99147	1.44E-05

What are x_+ and x_- for iteration 18?

What is x_{new}?

Bisection Evaluation

- Slow to reach accurate solution
- Does not make use of function values
  - First iteration had very low value of $f(x_{new})$ indicating that this guess was close to root, but only the sign of this root was used
  - There are times when the iteration keeps one value x_+ or x_- the same for several iterations
- But, this method will always converge; it will only blow up if there is a discontinuity

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Newton's Method

- Based on taking two terms in a Taylor series $f(x) = f(x_k) + (df/dx)_{x=xk} (x - x_k)$
- Solve this series approximation for x_{k+1} that sets $f(x) = 0$
  - $0 = f(x_k) + (df/dx)_{x=xk} (x_{k+1} - x_k)$

$$x_{k+1} = x_k - \frac{f(x_k)}{(df/dx)_{x=x_k}}$$

- Newton's method requires only one initial guess, but it requires the evaluation and calculation of the derivative

Newton's Method II

- Make one initial guess, x_0
- Repeat the following step to get a new guess, x_{k+1}, from the old guess, x_k
  - Compute x_{k+1} from the following equation

$$x_{k+1} = x_k - \frac{f(x_k)}{(df/dx)_{x=x_k}}$$

- Continue iteration until the value of x_{k+1} and/or $f(x_{k+1})$ is sufficiently accurate

Newton's Method III

- Find root of $f(x) = 0.05x - \sin(x)$ between x = 2 and x = 4
- For this f(x), $df/dx = 0.05 - \cos(x)$
- The iteration equation becomes

$$x_{k+1} = x_k - \frac{f(x_k)}{(df/dx)_{x=x_k}} = x_k - \frac{0.05x_k - \sin(x_k)}{0.05 - \cos(x_k)}$$

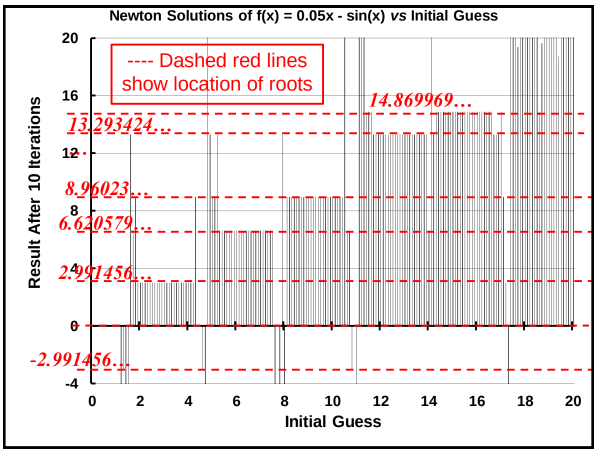
- For an initial guess $x_0 = 3$, $x_1 = 2.991461$

$$x_1 = x_0 - \frac{0.05x_0 - \sin(x_0)}{0.05 - \cos(x_0)} = 3 - \frac{0.05(3) - \sin(3)}{0.05 - \cos(3)}$$

Newton's Method IV

$$x_2 = x_1 - \frac{0.05x_1 - \sin(x_1)}{0.05 - \cos(x_1)} = 2.99 - \frac{0.05(2.99) - \sin(2.99)}{0.05 - \cos(2.99)}$$

- Gives $x_2 = 2.99145643340241$
- Next: $x_3 = 2.99145643340038$ and $f(x_3) = 0$ so further iterations give same x
- Initial guess of 2 or 4 gives same result in five (5) iterations
- Get different roots with different initial guesses



Evaluation of Newton's Method

- Sometimes used in computer code for problems that have to be solved often
  - In these cases initial derivative calculation is small part of total work
  - Otherwise use of simpler methods (like secant method) are faster because there is no need to evaluate derivative there
    - Secant method is sometimes described as a Newton-like method where the derivative is estimated numerically rather than being calculated exactly as in Newton's method

False Position (*Regula falsi*)

- This method uses an linear expression for the new guess like the secant method

$$x_{k+1} = x_k - f(x_k)\frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

- Unlike the secant method, which uses the two most recent iterations, false position always uses the two most recent guesses **which bracket the root**

False Position Algorithm

- Start with two guesses x_+ and x_- that bracket a root with $f(x_+) > 0$ and $f(x_-) < 0$
  - Notation similar to bisection method
- Use modified version of secant interpolation algorithm that works with the two guesses that bracket the root to get new guess, x_{new} and $f_{new} = f(x_{new})$

$$x_{new} = x_+ - f(x_+)\frac{x_+ - x_-}{f(x_+) - f(x_-)} \qquad f_{new} = f(x_{new})$$

Algorithm Detail

- Repeat the following steps for the two current guesses x_+ and x_-
  - Use a linear interpolation (like the secant method) to get x_{new} and $f_{new} = f(x_{new})$

$$x_{new} = x_+ - f(x_+)\frac{x_+ - x_-}{f(x_+) - f(x_-)} \qquad f_{new} = f(x_{new})$$

  - If $f_{new} > 0$ replace x_+ by x_{new}
  - If $f_{new} < 0$ replace x_- by x_{new}
- Continue until iterations give desired accuracy for x or f

False Position Example

- Example: apply this algorithm to solve $f(x) = 0.05x - \sin(x) = 0$
  - Initial values x = 2, 4 from bisection
  - $f(2) = 0.05(2) - \sin(2) = -0.8093$, so $x_- = 2$
  - $f(4) = 0.05(4) - \sin(4) = 0.9568$, so $x_+ = 4$
  - Apply interpolation formula for first iteration

$$x_{new} = x_+ - f(x_+)\frac{x_+ - x_-}{f(x_+) - f(x_-)}$$

$$x_{new} = 4 - f(4)\frac{4-2}{f(4)-f(2)} = 4 - 0.9568\frac{4-2}{0.9568-(-0.8093)} = 2.916$$

$$f_{new} = f(2.916) = 0.05(2.916) - sin(2.916) = -0.007139$$

Will x_{new} replace x_+ or x_-?

False Position Algorithm II

- Apply algorithm rules
  - If $f_{new} > 0$ replace x_+ by x_{new}
  - If $f_{new} < 0$ replace x_- by x_{new}
- $f_{new} < 0$ so $x_{new} = 2.916$ replaces $x_- = 2$
- Retain previous value of $x_+ = 4$
- Continue iteration with these values

$$x_{new} = x_+ - f(x_+)\frac{x_+ - x_-}{f(x_+) - f(x_-)}$$

$$x_{new} = 4 - 0.9568\frac{4-2.916}{0.9568-(-0.007139)} = 2.998$$

$$f_{new} = f(2.998) = 0.05(2.998) - sin(2.998) = 0.006346$$

Will x_{new} replace x_+ or x_-?

False Position Iterations

x_+	x_-	$f(x_+)$	$f(x_-)$	x_{new}	$f(x_{new})$	Δx_{new}
4	2	9.568E-01	-8.0930E-01	2.91647977182172	-7.7392E-02	
4.0000	2.916479	9.568E-01	-7.7392E-02	2.99756336632598	6.3463E-03	-8.3739E-02
2.9976	2.916479	6.346E-03	-7.7392E-02	2.99141826018393	-3.9652E-05	6.3860E-03
2.9976	2.991418	6.346E-03	-3.9652E-05	2.99145641684829	-1.7194E-08	-3.9635E-05
2.9976	2.991456	6.346E-03	-1.7194E-08	2.99145643339340	-7.4547E-12	-1.7186E-08
2.9976	2.991456	6.346E-03	-7.4547E-12	2.99145643340057	-3.3584E-15	-7.4513E-12
2.9976	2.991456	6.346E-03	-3.3584E-15	2.99145643340058	0	-3.3584E-15

- False position takes more iterations than secant, but is less prone to error
  - Note that last four iterations give new value of x_- leaving same value for x_+

Successive Substitution

- Easiest algorithm, but very slow and may not converge
- Write equation in form x = g(x)
  - Example: to solve $e^x = \sin(x)$ we can write $x = \ln(\sin(x))$ or $x = \sin^{-1}(e^x)$
- Algorithm: Start with initial guess x_0
- Compute new guess, $x_{k+1} = g(x_k)$
- Repeat until two values of x are sufficiently close

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Successive Solution Example

- $0.05x = \sin(x)$ is $x = g(x) = 20\sin(x)$
- Take initial guess, $x_0 = 3$
  - $x_1 = 20\sin(x_0) = 20\sin(3) = 1.51\text{x}10^{-1}$
  - $x_2 = 20\sin(x_1) = 20\sin(1.51\text{x}10^{-1}) = 7.53\text{x}10^{-3}$
  - $x_3 = 20\sin(x_2) = 20\sin(7.53\text{x}10^{-3}) = 3.76\text{x}10^{-4}$
  - $x_4 = 20\sin(x_3) = 20\sin(3.76\text{x}10^{-4}) = 1.88\text{x}10^{-5}$
  - $x_5 = 20\sin(x_4) = 20\sin(1.88\text{x}10^{-5}) = 9.41\text{x}10^{-7}$
  - $x_6 = 20\sin(x_5) = 20\sin(9.41\text{x}10^{-7}) = 4.71\text{x}10^{-8}$
  - $x_7 = 20\sin(x_6) = 20\sin(4.71\text{x}10^{-8}) = 2.35\text{x}10^{-9}$

What is x_8? ***$20\sin(x_7) = 1.17\text{x}10^{-10}$***

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Successive Substitution

- Simplest method for a single step
- May take many steps to converge
- Limited range of convergence: must have $|dg/dx| < 1$ in vicinity of root
- For equation $ax = \sin(x)$ writing $x = g(x) = \sin(x)/a$ gives zero root (or diverges) for any initial guess
  - Writing equation as $x = g(x) = \sin^{-1}(ax)$ diverges for any initial guess, even root exact to 15 significant figures

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First Quiz Results

- Number of students: 20
- Maximum possible score: 25
- Mean: 19.5
- Median: 22
- Standard deviation: 6.52
- Grade distribution

```
  0 11 12 12 16 16 19
  20 22 22 22 23 23
 23 24 24 25 25 25 25
```

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Comments on Quiz

- Cannot use statements like following with ElseIf: `if x<0 Then y = 3`
- Do not use unnecessary $
- Can simplify ElseIf clauses using information from pervious conditions
- In VBA use log for natural logarithm
- Watch parens in 1/n+1 vs. 1/(n+1)

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