

MATLAB Programming for Numerical Computation
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Module No. #05

Lecture No. #5.1

Non-Linear Algebraic Equations - Nonlinear equation in single variable

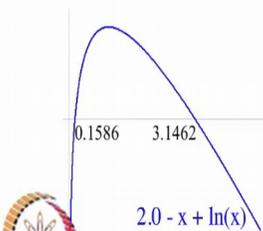
Hello and welcome to MATLAB programming for numerical computations. We are now, in week number 5. We are about the halfway mark, in this online course. In this week, we are going to cover nonlinear algebraic equations. In the first couple of lectures, we are going to cover nonlinear algebraic equations in a single variable, and finally we will cover nonlinear algebraic equations in multiple variables.

The first lecture, lecture 5.1, is going to be about, introduction to ourselves for nonlinear equations. And we will use, one simple method known as the Bisection method, in order to solve one, an example of nonlinear equation in a single variable.

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A Simple Example

To solve the following equation:

$$2.0 - x + \ln(x) = 0$$


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The solution is the location where the curve intersects the X-axis

It is possible to have multiple solutions (finite) to the problem

Computational Techniques: Module-4
<http://nptel.ac.in/courses/103106074/9>

So, the simple example that we are going to talk about today, is to solve the equation $2-x+\ln(x)=0$. Now if I am going to plot this function on the positive x axis, this is what the function is going to look like, the blue color line represents $2-x+\ln(x)$. Graphically, the solution to this

particular curve, is going to be nothing but, all the points that the curve intersects the x axis. Keep in mind that, while the solution that is going to be the solutions where the curve intersects the x axis; it is also possible to have multiple solutions as seen over here.

Unlike, the linear equations case, in linear equations, if the matrix A had is full rank matrix, then we can have only unique solution. However, in nonlinear equations case, we can have finite number of multiple solutions. If you recall from linear equations, whenever we had multiple solutions, we had infinite number of multiple solutions okay. So, that is going to be one difference between the linear algebra linear equations case and the nonlinear equations case.

The related set of lectures, in the computational techniques course is in module number 4 of computational techniques, the link for the first lecture is shown over here. So, you can go to that link, in order to find out some of the more theoretical stuff, related to solving nonlinear equations. What we are going to primarily do in this lecture series is, really take examples of solving nonlinear equations and solve them using MATLAB.

So, we are not going to derive any theory, but our primary focus is going to be on how to use MATLAB, in order to solve this nonlinear equation.

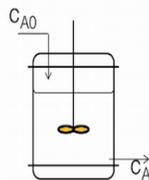
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General Setup

Let x be a variable of interest. The objective is to find the value of x which satisfies the following nonlinear equation:

$$f(x) = 0$$

Example: Model for a reactor



$$\frac{C_{A0}}{\tau} - \frac{C_A}{\tau} - \frac{kC_A}{(1+KC_A)^2} = 0$$

$f(C_A)$

So, the general setup, is going to be, let x be the variable of interest. And the objective is for to find the value of x , that satisfies the nonlinear equation $f(x) = 0$. An example for this is a model of a reactor and the model of the reactor follows an equation that is given below. In this example that x gets replaced by C_a and we are going to solve to obtain the concentration C_a , at the outlet of this reactor okay.

There are several other problems of interest, from various engineering discipline, as well as from various sciences. In this particular, set of lecture series, we are interested in solving, any generic equation of the sort $f(x) = 0$. When we talk about, a variable in a single variable, or a function in a single variable, we basically mean that x is a scalar valued variable, and f is a single scalar valued function.

In case of multivariable case, x is going to be an n dimensional vector, and our function f is actually not going to be a single function, but a vector of n functions, f_1, f_2 and so on up to f_n okay. So, let us now concentrate in the next couple of lectures, on solving the equations in single variable.

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The slide is titled "General Strategy of Solution" and features a small video inset of a speaker in the top right corner. The main content includes a graph of the function $2.0 - x + \ln(x)$ on the left, which is a downward-opening curve. A red double-headed arrow points to the x-axis, indicating the search for a root. To the right of the graph is a flowchart with the following steps: "Start with initial guess(es)", "Using a chosen strategy, move in the direction of the solution", and "Verify if stopping criterion is satisfied". A yellow arrow labeled "Yes" points down from the final step to the text "Solution!".

And the methodology that we are going to adopt, the general strategy that we are going to adopt is as follows okay. So when we have this particular curve, now keep in mind that, this curve how the curve looks like and so on, is typically not known to us a priori. This is a reasonably simple example, that we can actually plot the curve, and we can know how the curve looks like, but lot of times we may not be able to know how the curve looks like.

In that case, we are going to start with certain initial guess which is shown by this orange color dot over here okay. The choice of an initial guess is actually very important in nonlinear equations, something that has been covered in the computational techniques lecture series, which I mentioned a couple of slides earlier. You can refer to any standard textbook, in mathematics or in numerical methods. And you will be able, to know, what, how the initial guess has a profound impact on, how the solution evolves.

So we start with an initial guess, and this is going to be an iterative solution technique, just like the Gauss Siedel or the Jacobi iterations where, in module 3, excuse me, in module 4 okay. So we start with certain initial guess and we use a chosen method, chosen strategy, to move in the direction of the solution. So that direction of the solution, is shown by the brown arrow and the orange dot moves from its initial position to a new position okay.

Now, we actually check whether some kind of stopping criteria is satisfied or not. What start stopping criteria could be, is whether or not that change in x , is sufficiently large and that is the stopping criteria based on x , or whether $f(x)$ is sufficiently close to 0. So the stopping criteria, is either going to be from a graphical view point, whether this arrow, this brown color arrow is short enough, so that we can say, that we have reached close enough the solution or if this vertical distance is, short enough, so that we can say that, we are reasonably accurate, when it comes to solving the equation $f(x) = 0$.

Clearly in this particular geometry case we have not reached our desired solution. And, therefore we need to repeatedly solve these 2 steps over and over again. We use the same method to choose, to move further in the direction of the solution. Again, verify whether the stopping criteria is met. If the stopping criteria is met, we have our solution, if not we keep repeating these 2 steps over and over again okay. So, this is the methodology that we are going to implement in an example that I am going to cover next.

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Bisection Method (Single Variable Only)

- Start with two initial guesses, $x^{(l)}$ and $x^{(u)}$
- Verify that signs of $f(x^{(l)})$ and $f(x^{(u)})$ are different
- Repeat the following steps
 - New guess $x^{(new)}$ is the midpoint of the previous two guesses
 - Calculate $f(x^{(new)})$
 - Replace either $x^{(l)}$ or $x^{(u)}$ with based on sign of $f(x^{(new)})$

Related: Computational Techniques Module-4 Part-2: <http://nptel.ac.in/courses/103106074/10>

And that example, is going to be bisection method, in a single variable okay. So, this bisection method, is what is known as a, bracketing method, that means we do not start with a single solution. Unlike this figure, we are not going to start with a single solution, but we are going to start with 2 solutions. One of them is going to be, on one side of our actual solution, and the other guess is going to be on the other side of the actual solution.

Which means that, our $f(\text{guess } 1)$ and $f(\text{guess } 2)$ are going to have opposite signs okay. So, start with 2 initial guesses x_l and x_u , x lower bound and x upper bound. Verify that signs of x_l and x_u are different. So, in this case, let us say our f_l was going to be equal to 1, and our x_l was going to be equal to 1 and x_u was going to be equal to 4 okay. Then, first we verify, whether $f(1)$ is of a different sign than $f(4)$. If it is of a different sign, then those are permissible initial guesses okay.

And then, we choose the next guess, as nothing but the midpoint of the previous two guesses. So our x_{new} is going to be nothing but $(x_l + x_u) / 2$ okay. Then we calculate our $f(x_{new})$, and depending on where the sign is, we are going to either retain x_l or x_u . So, for example, our guesses are over here and over here are the initial guesses. The next is going to be, $(1+4) / 2$ which is 2.5. So, let us say that 2.5 is over here which is on the same side as x_l . So we drop x_l and x_{new} becomes our new x_l okay.

We continue that, and let us say our x , x_{new} again comes on the other side of this dot, which means on the same side of $x(u)$. In that case, we will drop x_u instead of x_l . And we keep doing that over and over again, in an iterative fashion, and that becomes our bisection method okay. The link, to the computational techniques module4, part2, is given over here. You can go to that link, to get and to understand, some of the theoretical aspects behind the bisection method okay.

So, let us head on over to MATLAB and try to solve the equation $2-x+\ln(x) = 0$, using bisection rule. Our initial guesses are going to be, $x(l) = 1$ and $x(u) = 4$. So, let us go on to MATLAB to solve this okay. (Video Starts: 09:51) edit bisecRule okay. Yes, open a new function, script file to use bisection method to solve $2-x+\log(x) = 0$ okay.

Initial guesses, $x_l = 1$, $x_u = 4$, f_l is going to be equal to $2-x_l+\log(x_l)$ and f_u is going to be equal to $2-x_u+\log(x_u)$. Check if signs, of f_l and f_u are different okay. So how do we check, whether the signs are different or not, we will just multiply f_l and f_u , if the signs are same the product f_l multiplied by f_u is going to be positive? So, if both f_l and f_u are positive, the sign is, of the product is going to be positive.

If both f_l and f_u are negative, again the sign is going to be positive. So therefore, we are going to multiply f_l and f_u , and check whether it is less than 0. If it is less than 0, we are good. If it is greater than 0, that means f_l multiplied by f_u is positive. Then we are not going to be, we know that f_l multiplied by f_u is positive, that means f_l and f_u have the same sign, so okay.

So, if $f_l * f_u$ greater than 0, then error, initial guesses should have different signs. And f_l multiplied by f_u is actually going to be less than 0. Then we are fine. So we do not need an else condition over here. Iterative solution using bisection okay. So, let us look at, so let us say error, is going to be equal to nothing but $\text{abs}(x_l - x_u)$. That is going to be our error, and let us say, we are now going to have our next solution. x_{new} is going to be $(x_l + x_u) / 2$ right. So, $(x_l + x_u) / 2$. So that is going to be our x_{new} okay.

What we want to check is, whether $f(x_{new})$ that is f_{new} whether that has the same sign or not. So f_{new} , is going to be $2-x_{new}+\log(x_{new})$ okay. So, let us check, the sign of f_{new} multiplied by f_l . If f_l multiplied by f_{new} is going to be greater than 0, which means f_l and f_{new} have the same sign, then $x_l = x_{new}$ and $f_l = f_{new}$, else x_u is going to be equal to x_{new} and $f_u = f_{new}$ and so this is one single iteration.

We need to iterate over this, but let us go on and run one single iteration and see whether that works or not okay. So let us go to MATLAB and say `bisecRule`. Let us hope, that we do not get an error. Let us press enter okay. So, it works for now okay. So now our `xu` is, so let us check what our `xl` is. `xl` is 2.5, `xu` is 4.0, our `f1` now is 0.4163 and our `fu` remains the same as negative 0.6137 okay. So, what has happened in this particular case is, we have run one single iteration okay of our bisection rule and in that single iteration of the bisection rule. (Video Ends: 15:02)

Now let us go on to power and see what has actually happened. So, we have moved from, this particular $x=1$ to a mid which is located somewhere over here okay. (Video Starts: 15:15) So now if you check the value of, $f(l)$ or $f(u)$, they are still sufficiently far away from 0. Or if you check the distance between `xu` and `xl`, we still have a very large distance between `xu` and `xl`. So therefore we conclude that our iteration has not converged.

So, let us go on and run this for one more iteration. So, I will just go on into this section, right click and I will say, evaluate current section. We can do this sectioning, because we have used a double percentage sign over here okay. If we do not use, that sectioning, it is not possible we can then instead, highlight this entire passage. Right click on this, and say evaluate current, sorry evaluate selection. So, the selected part, will be evaluated again, or we can just go over here and say evaluate this section.

So, evaluate current section, which means only these commands are going to be reevaluated, and let us see what our `xl` and `xu` are. Now `xl` remains 2.5, our `xu` has changed from 4 to 3.25, now 3.25 is the midpoint between 4 and 2.5 okay. And our `f1`, if we check, will remain the same as before 0.4163 and if we check `fu`, now `fu` would have changed and if `fu` has become -0.0713.

So, let us go to MATLAB and do this in a loop. So, for now, I will just do this in a for loop okay. So, for `i=1: maxIter`, where `maxIter` basically means max iteration. So, let us say `maxIter` equal to say 50. Let us run this for 50 iterations okay. Let us select this, right click and say smart indent. Smart indent means. The entire set of code will get beautified and we will go at the end and press end okay. So, we now have created this in a loop and in a for loop and we want to check the errors okay. So save this and error, keep in mind is nothing but abs value of `xl-xu` okay. And let us run this. Let us see if we get an errors okay.

There are no errors okay. And what do we have over here is, err, which is the difference between the x_l and x_u is 10 to the power of -15 . So that is pretty small number. So that means, we should be extremely satisfied with our solution, and if we check our f_{new} , our f_{new} is also $1 \cdot 10$ to the power -15 . So, that means we are now very close, to the solution $f_x = 0$ as well okay. So we actually did not need 50 iterations. So let us go back and reduce the number of iterations to 25 and see how this works. So save this and run it.

Let us go over here, and check our error. err is nothing but difference between x_l and x_u which will give us, a tolerance in our solution, that we want in the solution x that we want and that error is 10 to the power -7 and f_{new} which is trying to see how close our solution is to 0, is 10 to the power -8 . So, I think with this also it is a sufficient amount of convergence. (Video Ends: 19:07) So let us go back to our PowerPoint and see what we have done. So we have solved this using bisection method right. Now we have kind of solved it in a naïve way, not in a very polished way. We will change this in the next lecture okay.

However, what we have done is, we demonstrate the core principle of any non-linear equation solving, that we start with an initial guess or a set of initial guesses. And we use a chosen strategy, to the move in the direction of the solution. In this case, that the case of bisection method, the movement in the direction of the solution, was taking the average between the 2 guesses x_l and x_u . And checking whether the stopping criteria is satisfied. The last part, we have not yet done, that is something that we would do in the next lecture okay.

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Methods to Solve Nonlinear Equations



- Bracketing Methods
 - Bisection method
 - Regula Falsi
- Open Methods
 - Secant method
 - Fixed-point iteration
 - Newton-Raphson
- MATLAB functions `fzero` and `fsolve`

Methods that to solve nonlinear equations, that were covered in computational techniques module 4. Where, Bisection and Regula Falsi methods were bracketing methods, Secant, Fixed Iteration and Newton Raphson were the open methods. We are not going to cover, all the methods. We do not intend to be exhaustive in covering all the methods. But we want to cover the most important of the methods. The most important bracketing methods in my opinion is the bisection method that is also the method that is used partly that is used in the MATLAB function `fzero`, and then we have open methods which were fixed iteration and Newton Raphson method.

Fixed iteration, is kind of similar to the Gauss Seidel method that we saw in the previous module. Newton Raphson method is one of the most popular methods to solve nonlinear equations, and a related MATLAB method is known as `fsolve`, which uses a very different sort of algorithm, in order to solve the equations. We will not go into the algorithm for `fsolve`, but we are going to primarily use MATLAB functions `fzero` and `fsolve` as well. So that is going to be our strategy in the next 5 or 6 lectures of this module.

We are going to talk about Fixed Point Iteration and Newton Raphson method in single variable. We are going to talk about how to use `fzero` method in order to get solution. We are then going to talk about multivariate Newton Raphson method and multivariate Fixed Iteration method and finally end with using `fsolve`. In order to solve a sequence of nonlinear equations, n nonlinear equations and n unknowns and that is going to be the strategy for module 5. So with that I come to the end of the lecture 5.1. I will see you in the next lecture.