ChEE 201
Fall 2005
University of Arizona
Computer Reading 4
Taylor Series Approximations

Students learned a little bit about errors in the last reading so we are now ready to discuss the Taylor Series approximation, which is often a very useful tool for transforming a complex non-linear function into a linear equation so we can solve systems of larger equations that have the same variables. This technique is very useful in numerical methods, transport phenomena, and in chemical engineering controls. In addition, the techniques from this section will be used when we discuss non-ideal gases in chapter 5 of Felder and Rousseau.

Learning Objectives:
At the end of this section, students will be able to:
1) use the Taylor series expansion to represent a function as a linear expansion
2) understand how the approximate relative error can be used to decide when they have included enough terms in their infinite series to have come close enough to a converged answer to stop adding new terms

The Taylor series is extremely useful if you want to find the answer to a mathematical function but don't have a calculator. It's also useful when you need to solve a complex or non-linear equation and can come up with a good guess for a starting point. With that said, we could start off with a long boring derivation about where the Taylor series comes from. Instead, let's jump in with the formula and describe what is happening:

$$f(x_{i+1}) \approx f(x_i) + \frac{f'(x_i)}{1!}(x_{i+1}-x_i) + \frac{f''(x_i)}{2!}(x_{i+1}-x_i)^2 + \cdots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1}-x_i)^n$$

Here, we will use x_i to represent the value that we know the function at. Let's say we wanted to know what the square root of 5 is. Well, we could choose x_i to be any number that we know the square root of, like x_i = 1, 4, 9, etc. In this case, $x_{i+1} = 5$. For this example, we'll set x_i to 4, which is very close to x_{i+1}. Later on in this section, we'll see what happens when we change x_i.

We could use just the first term of the Taylor series approximation and we'd have:

$$f(x_{i+1}) = \sqrt{5} \approx \sqrt{4} = 2$$

So, here we're saying that the square root of 5 is close to 2. Well, we know that's not right because the square root of five is slightly higher. Let's now add the next term to our Taylor series approximation. Recall that:

$$\sqrt{x} = x^{\frac{1}{2}}$$

So the first derivative is:

$$f'(x) = \frac{1}{2}x^{-\frac{1}{2}} = \frac{1}{2x^{\frac{1}{2}}} = \frac{1}{2\sqrt{x}}$$

And now we evaluate this at x_i to get:

$$f'(x_i) = \frac{1}{2\sqrt{x}} = \frac{1}{2\sqrt{4}} = \frac{1}{4}$$

Let's now plug our information into the Taylor series for the first two terms:

$$f(x_{i+1}) = \sqrt{5} \approx \sqrt{4} + f'(x_i)\left(\frac{x_{i+1}-x_i}{1!}\right)$$

$$\sqrt{5} \approx 2 + \frac{1}{4}\frac{1}{1!}(5-4) = 2 + \frac{1}{4}(1) = 2.25$$

So, we've moved closer to what the final answer should be, but we probably aren't close enough to the final real answer to stop. Let's now add the next term, which has the second derivative of the function in it. We won't show quite as much math this time, but we find that our third derivative is:

$$f''(x) = \frac{1}{2}\left(-\frac{1}{2}\right)x^{-\frac{3}{2}} = -\frac{1}{4x^{\frac{3}{2}}}$$

We plug this in and evaluate it at $x_i = 4$ to get the following:

$$\sqrt{5} \approx 2.25 + -\frac{1}{4(4)^{\frac{3}{2}}}\frac{1}{2!}(5-4)^2$$

where we just replaced the first two terms by what we had found in the previous step. Now we are trying to do this by hand so we recall that:

$$x^{\frac{3}{2}} = x^{\frac{2}{2}}\left(x^{\frac{1}{2}}\right) = x\left(x^{\frac{1}{2}}\right)$$

Our Taylor series then becomes:

$$\sqrt{5} \approx 2.25 - \frac{1}{4(4)(4)^{\frac{1}{2}}}\frac{1}{2}(1)^2 = 2.25 - \frac{1}{16(2)2} = 2.25 - \frac{1}{64}$$

$$\sqrt{5} \approx \frac{9}{4} - \frac{1}{64} = \frac{144-1}{64} = \frac{143}{64}$$

We could have used a calculator if we wanted to, but we didn't have to. Notice that the first term was the largest of the three, while each successive term got smaller and smaller. Let's now turn to our calculator and see how we've done so far. Our approximate answer after three terms is 2.234375. Using our calculator, the square root of five is 2.236067977. Our true error is 0.001692, while the true fractional error is 0.000757, which is very good for not using a calculator until the final step. If we added more terms, we wouldn't really improve our answer that much more so we could stop here. If we didn't have the true answer to compare to, how would we know we could stop?

Recall from the error discussion in the previous section that even if we don't know the true answer, we can calculate the approximate error and the approximate relative error. We can't do it for the first term, but we can after finding the second and larger terms in the series. After we added the first derivative term our errors were:

$$E_a = 2.25 - 2.00 = 0.25$$

$$E_{a,relative} = \frac{0.25}{2.25} = 0.111$$

And after adding the second derivative term we found our errors were:

$$E_a = 2.23438 - 2.25 = -0.01562$$

$$E_{a,relative} = \frac{-0.01562}{2.23438} = -0.00699$$

Recall that we said we can often choose a stopping criteria when the newest terms lead to a fractional error with an absolute value of 0.01-0.05, or around a few percent, depending on how important the accuracy is in our final number.

Now that we have the basic mechanics of how to use a Taylor series approximation, including how to use the approximate relative error to stop when we think our answer is accurate enough, let's look at some of the other details of how to best use the Taylor series.

Choosing x_i wisely:

The first caveat to remember when choosing x_i is to choose it such that you know what the function equals for that value. This is why we wouldn't have chosen x_i to be 7...because we don't necessarily know what the square root of seven is!

The farther x_i is from x_{i+1} where we want to know the value, though, the longer it will take for our approximation to converge to an answer, requiring more terms. Let's look at finding the square root of 5 by using x_i values of 4, 9, and 25. We'll make a table that has the x_i guess on the top of the columns while we calculate the function's value and approximate relative error as we go down the table. This is shown here:

x_i guess	4		9		25	
terms included	value	approximate relative error	value	approximate relative error	value	approximate relative error
1	2.00000		3.00000		5.00000	
2	2.25000	0.11111	2.33333	-0.28571	3.00000	-0.66667
3	2.23438	-0.00699	2.25926	-0.03279	2.60000	-0.15385
4	2.23633	0.00087	2.24280	-0.00734	2.44000	-0.06557
5	2.23602	-0.00014	2.23823	-0.00204	2.36000	-0.03390

We see that when x_i was close to x_{i+1} (4 with 5), we had very fast convergence and the approximate relative error quickly dropped to less than 0.01 by the third term. In contrast, as we move x_i farther from x_{i+1} and use 9, we see it takes another term to be added to get under 0.01. And when we're even farther away at 25, we still haven't converged after five terms.

So, you see that having x_i and x_{i+1} close together helps us get to a solution faster.

<u>Being careful with math:</u>
It is very common for students to make errors when they are taking their derivatives and when they are putting all their results into their Taylor series formula. So, here are some things that you should look out for:

- Make sure you are taking the derivatives of the functions and NOT using the integrals instead
- Be careful of your signs as you include them in your formulas
- Don't forget to include the powers on the difference terms (x_{i+1}-x_i)
- And don't forget to include your factorials in the denominator

If you would like some practice, try the following problem:
Find e^1 without using a calculator.

If you are having a hard time getting started, go through the following steps:
1) Identify x_{i+1}
2) Choose an x_i that you know the function for without using a calculator
3) Take the first 2 to 3 derivatives
4) Evaluate the derivatives with xi plugged in
5) Compute the Taylor series terms
6) Add up enough terms until your approximate relative error is less that 1% (0.01).

There are three types of procedures that help engineers reach correct answers:

- be methodical
- be orderly in the way you organize information
- check your work

If you'd like to see how this is done, check the next page where you can fill in the blanks.

Fill in the following blanks:

x_{i+1} = x_i =

f(x) = evaluated at x_i =

f'(x) = evaluated at x_i =

f''(x) = evaluated at x_i =

$F^{(3)}(x)$ = evaluated at x_i =

Taylor series and the terms:

$$f(x_{i+1}) \approx f(x_i) + \frac{f'(x_i)}{1!}(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \cdots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n$$

$f(x_{i+1})$=

Final answer and error analysis:

For the solution as worked out by the instructor, go to the next page and compare to your work here. Keep in mind that all of the exercises in the readings are designed to help students master the material. If a student comes to office hours with a question about Taylor series, they will be asked to produce this sheet and work through it so it can be used to help figure out where they are having problems.

$x_{i+1} = 1$ $x_i = 0$

$f(x) = e^x$ evaluated at $x_i = 1$

$f'(x) = e^x$ evaluated at $x_i = 1$

$f''(x) = e^x$ evaluated at $x_i = 1$

$F^{(3)}(x) = e^x$ evaluated at $x_i = 1$

Taylor series and the terms:

$$f(x_{i+1}) \approx f(x_i) + \frac{f'(x_i)}{1!}(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \cdots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n$$

$$f(x_{i+1}) \approx 1 + \frac{1}{1!}(1-0) + \frac{1}{2!}(1-0)^2 + \frac{1}{3!}(1-0)^3 + \frac{1}{4!}(1-0)^4 + \frac{1}{5!}(1-0)^5 + \cdots$$

$$f(x_{i+1}) \approx 1 + 1 + \frac{1}{2} + \frac{1}{6} + \frac{1}{24} + \frac{1}{120} + \cdots$$

$$f(x_{i+1}) \approx \frac{240}{120} + \frac{60}{120} + \frac{20}{120} + \frac{5}{120} = \frac{325}{120} = 2.708333$$

The actual answer is 2.71828 so we were getting pretty close

Final answer and error analysis: (This part won't be filled in since you have worked through the errors on a homework already and should understand how to use them.)

Now that you've read this section, you're ready to tackle Computer Homework 4 online.