Mech 221 Mathematics Component

Differential Equations

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Lectures 1-4

Outline

Outline

Course Overview

Last Year:

Math 100: Differential Calculus

Math 101: Integral Calculus

Math 152: Linear Systems

This Term: carry on with two main ideas from last year.

- Numerical Approximation (carrying on from numerical integration in Math 101). *Riemann Sums, Trapezoidal Rule, Simpson's Rule.*
- Differential Equations (carrying on from DEs in Math 101 and 152). *Exponential growth and decay, separable equations, second order linear constant coefficient equations (auxiliary equation), method of undetermined coefficients, systems of linear equations (linear, constant coefficient, diagonalizable).*

Course Overview-II

You need to know how to Do the Math:

1. Convert an Engineering problem to a mathematical one (with simplifications).
2. Solve the mathematical problem.
3. Relate the mathematical solution to the original Engineering problem (with appropriate scepticism).

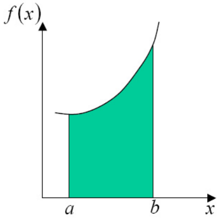
Why? Solving the problem with pencil and paper (and computations) rather than extensive physical design cycles is faster and cheaper.

Integration

Graphical Interpretation

Integral of a function is the area A under its graph

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

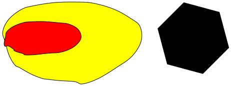


Applications of Integration: *average values, volumes, work, arc length, centre of mass, solving separable DEs.*

Integration-II

New Application

How much heat Q (in J) does it take to heat up a rock of mass M from 25° C to 1000° C?



If the thermal heat capacity c (in $J/kg/^\circ C$) *does not* depend on temperature, then

$$Q = cM(1000 - 25)$$

(makes sense and the units check out).

If the thermal heat capacity $c(T)$ (in $J/kg/^\circ C$) *does* depend on temperature, then

$$Q = M \int_{25}^{1000} c(T) dT.$$

Integration-III

New Application (cont.)

Derivation of

$$Q = M \int_{T_0}^{T_1} c(T)dT$$

Integration-IV

New Application (cont.)

Integration-V

Analytic Integration Review

Can you evaluate the following simple integrals?

$$\int_0^1 \sin x dx$$

$$\int e^{-x} dx$$

$$\int x e^{x^2} dx$$

$$\int x \cos x dx$$

Integration-VI

Analytic Integration Example

$$\int x \cos x dx$$

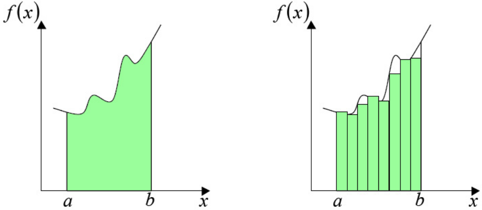
Numerical Integration

Left Riemann Sums

Some integrals cannot be evaluated analytically. Some functions are only known at a finite array of points (corresponding to experimental measurements). Use numerical methods.

If the interval $[a, b]$ is divided into N subintervals of length $h = (b - a)/N$, we can use the Left Riemann sum approximation

$$I = \int_a^b \approx L_N = hf(a) + hf(a + h) + hf(a + 2h) + \cdots + hf(a - h)$$



Numerical Integration

Left Riemann Sums

As $N \to \infty$ we know $L_N \to I$ (definition of the integral). Error made is

$$I - L_N = -\frac{f'(\xi)}{2}(b-a)h$$

where ξ is a point in $[a, b]$ (that is not known).

Numerical Integration-II

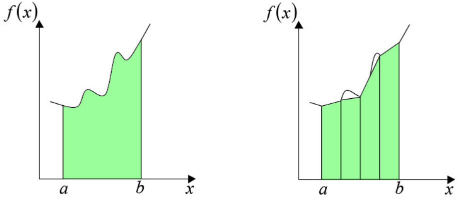
Trapezoidal Rule

We know from Math 101 we can get more accurate answers using other numerical integration methods.

$$I \approx T_N = \frac{h}{2}f(a) + hf(a+h) + hf(a+2h) + \cdots + hf(b-h) + \frac{h}{2}f(b)$$

with error expression

$$I - T_N = -\frac{f''(\xi)}{12}(b-a)h^2$$



Numerical Integration-III

Simpson's Rule

N must be even

$$
\begin{aligned}
I \approx S_N \quad = \quad & \frac{h}{3} f(a) + \frac{4h}{3} f(a+h) + \frac{2h}{3} f(a+2h) + \frac{4h}{3} f(a+3h) + \\
& \frac{2h}{3} f(a+4h) + \cdots + \frac{4h}{3} f(b-h) + \frac{h}{3} f(b)
\end{aligned}
$$

with error expression

$$
I - S_N = -\frac{f^{(4)}(\xi)}{180}(b-a)h^4
$$

Numerical Integration-IV

Doing the Computations

Take as an example:

$$\int_0^1 \sin x dx$$

Work out L_4, T_4, S_4.

Numerical Integration-V

Doing the Computations (cont.)

Numerical Integration-VI

Performance of Methods

$$\int_0^1 \sin x dx = 1 - \cos(1) \approx 0.4597$$

N	$I - L_N$	$I - T_N$	$I - S_N$
2	0.2200	0.0096	1.6×10^{-4}
4	0.1076	0.0024	1.0×10^{-5}
8	0.0532	0.00060	6.2×10^{-7}
16	0.0264	0.00015	
32	0.0132	0.00004	

Numerical Integration-VII

Direction

- Where do the error expressions come from?
- How could we work out how to get that accurate method (Simpson's rule)? *So we can get figure out how to get accurate numerical methods for other things*.

Outline

Taylor Polynomials and Series

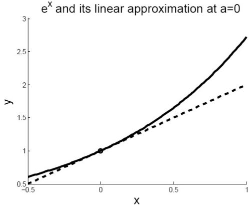
Linear Approximation

For x near a we have the linear (tangent line) approximation:

$$f(x) \approx f(a) + f'(a)(x - a)$$

As an example, take $a = 0$ and $f(x) = e^x$ to get the linear approximation

$$e^x \approx 1 + x$$



Taylor Polynomials and Series-II

Quadratic Approximation

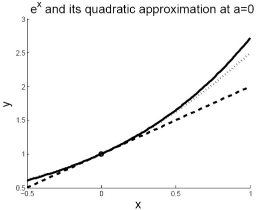
A better approximation is the quadratic one

$$f(x) \approx f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2$$

Note that the values, derivatives and second derivatives of the function and its approximation are the same at $x = a$.

Considering $a = 0$ and $f(x) = e^x$ again we get the quadratic approximation

$$e^x \approx 1 + x + \frac{x^2}{2}$$



Taylor Polynomials and Series-III

Taylor Quadratic Example

Find the quadratic Taylor approximation of $\arctan x$ based at $a = 1$.

Taylor Polynomials and Series-IV

Taylor Polynomial Approximation

Higher order (n) polynomial approximation ($P_n(x)$) can also be used:

$$f(x) \approx P_n(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n$$

Error formula

$$f(x) - P_n(x) = R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}$$

where ξ is a point between a and x (that is not known).

Taylor Polynomials and Series-V

Taylor Series

In some cases, $P_n(x) \to f(x)$ as $n \to \infty$. The "infinite" order polynomial is called a Taylor Series. Some common series are given below (based at $a = 0$, they can also be called McLaurin Series):

$$
\begin{aligned}
\sin x &= x - \frac{x^3}{6} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots \\
\cos x &= 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \\
e^x &= 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{4!} + \cdots \\
\frac{1}{1-x} &= 1 + x + x^2 + x^3 + \cdots \quad \text{for } |x| < 1
\end{aligned}
$$

Some Proofs

Rolle's Theorem

If f is differentiable, $f(a) = 0$ and $f(b) = 0$ then there is a point ξ in (a, b) at which $f'(\xi) = 0$.

Some Proofs-II

Rolle's Theorem (cont.)

Some Proofs-III

Error Estimate for Tangent Line Approximation

Show that

$$f(b) - [f(a) + f'(a)(b-a)] = \frac{f''(\xi)}{2}(b-a)^2$$

for some ξ in (a, b).

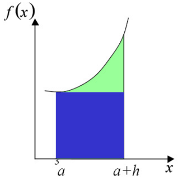
Some Proofs-IV

Error Estimate for Tangent Line Approximation (cont.)

Errors from Numerical Integration

Left Riemann Sums

Consider just one subinterval:



Using a Taylor polynomial and remainder argument, it can be shown that

$$\int_a^{a+h} f(x)dx - hf(a) = \frac{f'(\xi)}{2}h^2$$

where ξ is in $[a, a+h]$. Now sum over all subintervals (N subintervals length $h = (b-a)/N$):

$$\int_a^b f(x)dx - L_N = \frac{1}{2}(f'(\xi_1) + \cdots f'(\xi_j) + \cdots f'(\xi_N))h^2$$

where each ξ_j is in the j'th subinterval $[a + (j-1)h, a + jh]$.

Errors from Numerical Integration-II

Left Riemann Sums cont.

We had summed over all subintervals (N subintervals length $h = (b-a)/N$):

$$\int_a^b f(x)dx - L_N = \frac{1}{2}\frac{1}{N}(f'(\xi_1) + \cdots f'(\xi_j) + \cdots f'(\xi_N))(b-a)h$$

Note that an average of values of a continuous function on an interval is attained at a value in the interval (fancy application of the intermediate value theorem):

$$\int_a^b f(x)dx - L_N = \frac{1}{2}f'(\xi)(b-a)h$$

Careful consideration of the argument shows that

$$\int_a^b f(x)dx - L_N \approx \frac{h}{2}\int_a^b f'(x)dx = \frac{h}{2}(f(b) - f(a))$$

Is this a surprise?

Errors from Numerical Integration-III

Left Riemann Sums cont.

Consider the error expression applied to our example from last time:

$$\int_0^1 \sin x dx$$

We know that

$$\frac{d}{dx} \sin x = \cos x \text{ and } |\cos x| \leq 1 \text{ on } [0,1]$$

so the error bound is

$$\left| \int_0^1 \sin x dx - L_N \right| \leq \frac{1}{2} h = \frac{1}{2N}$$

The error estimate is

$$\int_0^1 \sin x dx - L_N \approx \frac{h}{2}(sin(1) - 0) = \frac{sin(1)}{2N}$$

smaller than error bound - check.

Errors from Numerical Integration-IV

Left Riemann Sums Example

Comparison of errors, error bounds, and theoretical estimates of the error.

N	$I - L_N$	Bound	Estimate
2	0.2200	0.2500	0.2104
4	0.1076	0.1250	0.1052
8	0.0532	0.0625	0.0526
16	0.0264	0.0313	0.0263
32	0.0132	0.0156	0.0132

Errors from Numerical Integration-V

Higher Order Methods

Local estimates:

$$\int_a^{a+h} f(x)dx - \frac{h}{2}(f(a) + f(a+h)) = -\frac{1}{12} f''(\xi) h^3$$

$$\int_a^{a+2h} f(x)dx - \frac{h}{3}(f(a) + 4f(a+h) + f(a+2h)) = -\frac{1}{180} f^{(4)}(\xi) h^5$$

where ξ is in $[a, a+h]$ (different value in the two expressions).

Technical, but the idea is that if the integration formula is exact for polynomials of order n, it's local errors behave like h^{n+2} and the total errors like h^{n+1}.

How would you derive a higher order method than Simpson's Rule?

Errors from Numerical Integration-VI

Final Discussion

Consider doing numerical integration on

$$\int_0^1 f(x)dx$$

where $f(x)$ has the following forms:

$$\begin{aligned}
f(x) &= e^{x^2}(\text{exact integral not known}) \\
f(x) &= \begin{cases} \sin(2x^2) \text{ for } x \leq 1/\sqrt{2} \\ \sin\left(\frac{1}{2x^2}\right) \text{ for } x > 1/\sqrt{2} \end{cases} \\
f(x) &= \frac{\cos x}{\sqrt{x}}(\text{singular integrand})
\end{aligned}$$

Outline

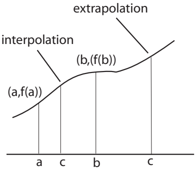
Interpolation

Interpolation and Extrapolation

Suppose you know the value of $f(a)$ and $f(b)$ and wanted to estimate the value of $f(c)$.

If c is in $[a, b]$ then this is called *interpolation*.

If c is outside $[a, b]$ then this is called *extrapolation*.

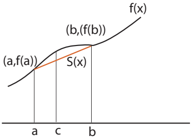


Note: This is *not* the same idea as least squares line fitting.

Interpolation-II

Linear Interpolation

Idea: Approximate $f(x)$ by the line segment between $(a, f(a))$ and $(b, f(b))$.



$$f(x) \approx S(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

so

$$\begin{aligned} f(c) &\approx f(a) + \frac{f(b) - f(a)}{b - a}(c - a) \\ &= \frac{b - c}{b - a} f(a) + \frac{c - a}{b - a} f(b) \end{aligned}$$

Interpolation-III

Example I

Vapour saturation pressure $P_{sat}(T)$ where P_{sat} is in bar and T is in $^\circ$C. Steam tables:

$$
\begin{aligned}
P_{sat}(25) &= 0.03168 \\
P_{sat}(30) &= 0.04241
\end{aligned}
$$

What is a good estimate of $P_{sat}(27)$? Use linear interpolation.

Interpolation-IV

Questions

Questions:

- How accurate is linear interpolation?
- How could we interpolate more accurately?
- If we use $S(x)$ for extrapolation, how big are the errors we make?

Interpolation-V

Linear Interpolation Error

Interpolation/Extrapolation error using $(a, f(a))$ and $(a + h, f(a + h))$:

$$f(x) - S(x) = \frac{1}{2}(x - a)(x - (a + h))f''(\xi)$$

(makes sense).

Interpolation error bound:

$$|f(x) - S(x)| \leq \frac{h^2}{8} \max_{s \in [a, a+h]} |f''(s)|$$

The proof is an assignment question.

Interpolation-VI

Example II

Say you knew from tables that

$$\begin{aligned} \sin(0.9) &= 0.7833 \\ \sin(1) &= 0.8415 \end{aligned}$$

And you wanted to estimate $\sin(0.95)$. Use linear interpolation:

$$\sin(0.95) \approx \frac{1}{2}(\sin(0.9) + \sin(1)) = 0.8124$$

Exact $\sin(0.95) = 0.8134$, error ≈ 0.0010.

Error bound above is

$$\frac{0.1^2}{8}\sin(1) = 0.00105$$

Extrapolation is much less accurate. Using $\sin(0.9)$ and $\sin(1)$ to estimate $\sin(0.8)$ gives an error of 0.0077.

Fancy Interpolation

Quadratic Interpolation

If we knew the values of $f(a-h)$, $f(a)$, $f(a+h)$ we could get a more accurate interpolation in $[a-h, a+h]$.

Idea: Use a quadratic approximation that has the same values as f at the points $x = a-h, a, a+h$.

$$Q(x) = c_0 + c_1 x + c_2 x^2$$

The coefficients are chosen so that

$$\begin{aligned} Q(a-h) &= c_0 + c_1(a-h) + c_2(a-h)^2 = f(a-h) \\ Q(a) &= c_0 + c_1 a + c_2 a^2 = f(a) \\ Q(a+h) &= c_0 + c_1(a+h) + c_2(a+h)^2 = f(a+h) \end{aligned}$$

It's a linear system for c_0, c_1 and c_2! Could solve for the coefficients, then use $Q(x)$ to approximate $f(x)$.

Fancy Interpolation-II

Quadratic Interpolation (cont.)

In fact, there is an easier way to construct $Q(x)$:

$$\begin{aligned} Q(x) &= \frac{(x-a)(x-(a+h))}{2h^2} f(a-h) \\ &+ -\frac{(x-(a-h))(x-(a+h))}{h^2} f(a) \\ &+ \frac{(x-(a-h))(x-a)}{2h^2} f(a+h) \end{aligned}$$

The terms multiplying the values of f are called Lagrange interpolating polynomials. Notes:

- The three points for quadratic interpolation do not have to be equally spaced.
- The error bound is $Ch^3 \max |f^{(3)}|$.
- Cubic and higher order interpolation can be done similarly.
- Interpolation formulae that are exact for order n polynomials have errors of order h^{n+1}

Fancy Interpolation-III

Fancy Interpolation Example

Experimental measurements determine that a function $f(x)$ satisfies $f(0) = 1$, $f'(0) = 1$, and $f(1) = 3$. Estimate $f(1/2)$ using

(a) tangent line approximation.

(b) linear interpolation.

(c) a quadratic interpolation using all the information.

Fancy Interpolation-IV

Fancy Interpolation Example (cont.)

Richardson Extrapolation

Recall that

$$I - T_n \approx \frac{C}{N^2}$$

and a theoretical study like we did for Left Riemann sums shows that

$$C = -\frac{(b-a)^2}{12}\int_a^b f''(s)ds$$

so

$$T_N \approx I - \frac{C}{N^2} \text{ and } \quad T_{2N} \approx I - \frac{C}{4N^2}$$

Notice that if we take

$$\frac{4}{3}T_{2N} - \frac{1}{3}T_N \approx I + \text{ (higher order error)}$$

So the combination rule $\frac{4}{3}T_{2N} - \frac{1}{3}T_N$ is much more accurate. It is in fact Simpson's rule S_{2N}.

Richardson Extrapolation-II

Another look at Richardson Extrapolation

Richardson Extrapolation-III

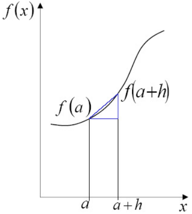
Another look at Richardson Extrapolation (cont.)

Outline

Differentiation

The derivative of a function is given as

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$



Graphical Interpretation of Derivative: the tangent line slope.

Applications of Derivatives: *approximation, related rates, optimization, differential equations*

Numerical Differentiation-II

Euler difference methods

$$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

Idea: take h small in the formula above (secant line slope approximation to the tangent line slope).

Forward Euler Difference Approximation:

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}$$

Backward Euler Difference Approximation:

$$f'(a) \approx \frac{f(a) - f(a-h)}{h}$$

Numerical Differentiation-III

Example

Approximate

$$\frac{d}{dx}\sin x$$

at $x = 1$ using $h = 0.1$ using FE and BE.

Numerical Differentiation-IV

Example (cont.)

Consider again the approximation of

$$\frac{d}{dx}\sin x$$

at $x = 1$. (exact value $\cos 1 = 0.5403$).

h	FE	FE error	BE	BE error
1/10	0.4974	0.0429	0.5814	-0.0411
1/20	0.5190	0.0213	0.5611	-0.0208
1/40	0.5297	0.0106	0.5508	-0.0105
1/80	0.5350	0.0053	0.5455	-0.0052
1/160	0.5377	0.0026	0.5429	-0.0026

Note that errors decrease by 2 when h is halved (first order methods) and that the errors for BE are almost equal in magnitude but opposite in sign to those of FE.

Numerical Differentiation-V

Centred Differencing

We would have a much more accurate approximation of the derivative if we averaged FE and BE (the error would approximately cancel).

$$f'(a) \approx \frac{1}{2}\frac{f(a+h)-f(a)}{h}+\frac{1}{2}\frac{f(a)-f(a-h)}{h} = \frac{f(a+h)-f(a-h)}{2h}$$

this is known as the centred difference formula.

Numerical Differentiation-VI

Error Estimates

The error estimates for difference formulae are easy to work out using Taylor Polynomials:

$$
\begin{aligned}
f'(a) - \frac{f(a+h) - f(a)}{h} &= -\frac{1}{2} h f''(\xi) \\
f'(a) - \frac{f(a) - f(a-h)}{h} &= \frac{1}{2} h f''(\xi) \\
f'(a) - \frac{f(a+h) - f(a-h)}{2h} &= -\frac{1}{6} h^2 f^{(3)}(\xi)
\end{aligned}
$$

Difference Formulae for first derivatives that are exact for order n polynomials have errors of order h^n

Numerical Differentiation-VII

Proof of Difference Formula

$$f'(a) - \frac{f(a+h) - f(a)}{h} = -\frac{1}{2} h f''(\xi)$$

Numerical Differentiation-VIII

Roundoff Errors and Noise

Consider using FE to approximate

$$\frac{d}{dx}\sin x = \cos x$$

at $x = 1$ (exact value $\cos 1 = 0.5403$) as before, but now take h to be very small.

h	FE error
10^{-4}	4.2e-5
10^{-6}	6.9e-7
10^{-8}	2.3e-6
10^{-10}	0.030

The last large error is due to roundoff in the floating point representation of numbers on my calculator.

Numerical differentiation is also very sensitive to noise in experimental data values.

More Difference Formulas

Example 1

Find the second order formula for $f'(a)$ when $f(a)$, $f(a-h)$ and $f(a-2h)$ are known.

More Difference Formulas-II

Example 1 (cont.)

More Difference Formulas-III

Example 2

Second order formula for $f''(a)$ when $f(a)$, $f(a-h)$ and $f(a+h)$ are known.

More Difference Formulas-IV

Example 2 (cont.)

Numerical Methods Summary

You now know how to approximate

- Integrals
- Derivatives
- Function values (interpolation)

using only discrete function values.