Introductory Lecture

- Many phenomena (physical, chemical, biological, etc.) are model by differential equations.
- Recall the definition of the derivative of $f(x)$ and its physical and graphical interpretation.

Example Suppose we are told that the population $p(t)$ of a colony of bird is only affected by their births and deaths. Then the change in the population is modeled by

$$\frac{dp}{dt} = r_b p - r_d p = \alpha p$$

where r_b denotes the rate of births, r_d denotes the rate of deaths, and $\alpha = r_b - r_d$. If we know the initial population p_0 at some time t_0 then we can find the *exact* population (based on our simplified model) at any later time. For example,

$$\frac{1}{p}dp = \alpha dt \Rightarrow \ln p = \alpha t + C \Rightarrow p = e^{C+\alpha t} = \hat{C}e^{\alpha t}$$

Using the fact that $p(t_0) = p_0$ gives $p = p_0 e^{\alpha t}$. If $\alpha > 0$ (i.e., more births than deaths) then the population grows; otherwise it declines.

This is a very simple model for which we can find an *analytic* solution. What if we change the model slightly by adding a migration term $M(t,p)$? For example $M(t,p) = e^{t \sin \pi p}$ then our approach above fails. How do we even know this problem has a solution? Even if we can demonstrate that it has a solution, we may not be able to find an analytic solution. What do we do if we can't find an analytic solution?

We must *discretize*. What does this mean? When we have an analytic solution we have a formula for every possible value of the independent variable (t in our example). When we discretize we typically approximate the solution at a finite number of points, say $t_1, t_2, \ldots, t_n$ and as $n \to \infty$ ($\Delta t \to 0$) we want our discrete solution to approach our analytic solution.

- We need to make precise what is meant by "approaching".
- What would happen if we try to discretize a problem that doesn't have a unique solution?

Example One way to discretize our problem above is to replace the derivatives by differences of function values. Recall that the derivative is defined in terms of the limit of a difference quotient of function values. So let's replace our derivative in the ODE with this difference quotient to see if we can approximate the solution $p(t^1)$ given its value at t_0.

$$\frac{p(t_1) - p(t_0)}{\Delta t} \approx \alpha p(t_0) + M(t_0, p(t_0))$$

where $\Delta t = t_1 - t_0$. Because we know $p(t_0) = p_0$ then

$$p(t_1) \approx p_0 + \Delta t \alpha p_0 + \Delta t M(t_0, p_0) = (1 + \Delta t \alpha)p_0 + \Delta t M_0$$

Everything on the right hand side is known so we can approximate $p(t_1)$. The procedure can be repeated. In general, we define a *discrete* function P^n which approximates $p(t_n)$. The general difference equation is then

$$\frac{P^{k+1} - P^k}{\Delta t} = \alpha P^k + M(t_k, P^k), \quad k = 0, 1, 2, \ldots$$

Notice where we use $=$ and $\approx$.

- We need to know that as $\Delta t \to 0$ then $P^k \to P(t_k)$.
- We would also like to know how fast P^k approaches $P(t_k)$ because if we have two methods which are the same amount of work, then if one approaches the exact solution faster than the other, we would feel that it is, in some sense, better.
- This type of problem is called an *initial value problem* (IVP).
- Can we apply this technique to any other IVP?

Example Consider the IVP

$$y'(t) = t\sqrt{y}, \quad y(0) = 0$$

which has a solution $y(t) = t^4/16$. (How do we know this? Clearly it satisfies the initial condition. We can check that it satisfies the equation by computing y' and substituting into the equation to see if we get equality, e.g.,

$$y' = \frac{4}{16}t^3 \qquad t\sqrt{y} = t(t^2/4) = t^3/4$$

Now our difference equation becomes

$$\frac{Y^{k+1} - Y^k}{\Delta t} = t^k\sqrt{(Y^k)} \Rightarrow Y^{k+1} = Y^k + \Delta t\, t^k\sqrt{(Y^k)}$$

Thus with $\Delta t = .1$

$$Y^1 = Y^0 + 0.1(0)\sqrt{0} = 0, \qquad Y^2 = Y^1 + 0.1(0.1)\sqrt{0} = 0, \ldots Y^k = 0$$

- What went wrong? $y = 0$ is also a solution of the problem; i.e., the solution of the IVP is NOT UNIQUE! Clearly we need to know if our original problem has more than one solution.

What do we do if we have an IVP where the DE has a higher derivative?

Consider the problem

$$u''(t) = t^2 \quad t_0 < t \leq 1$$

To solve this problem analytically we can just integrate twice to get

$$u'(t) = \frac{t^3}{3} + C_1 \Rightarrow u(t) = \frac{t^4}{12} + C_1 t + C_2$$

Note that because we have integrated twice we need two auxiliary conditions. For example, if $u(0) = 0$ and $u'(0) = 1$ we have $C_1 = 1$ and $C_2 = 0$ yielding $u(t) = \frac{t^4}{12} + t$.

- How do we obtain a difference equation for this DE?

  We need a difference quotient which approximates the second derivative.

- Taylors series is a useful formula for obtaining difference quotients. Recall that for small Δt and $u(t)$ possessing all derivatives Taylors series expansion for u in the neighborhood of t is

$$u(t + \Delta t) = u(t) + \Delta t u'(t) + \frac{\Delta t^2}{2!} u''(t) + \frac{\Delta t^3}{3!} u'''(t) + \cdots$$

  Note that this is an infinite series. We can also write the series in the remainder form, e.g.,

$$u(t + \Delta t) = u(t) + \Delta t u'(t) + \frac{\Delta t^2}{2!} u''(t) + \frac{\Delta t^3}{3!} u'''(t) + \frac{\Delta t^4}{4!} u''''(\xi), \quad \xi \in (t, t + \Delta t)$$

- Why is the second expression no longer an infinite series?
- How can we use Taylors series to obtain an approximation to $u''(t)$?

  Combining the above expression with

$$u(t - \Delta t) = u(t) + \Delta t u'(t) + \frac{\Delta t^2}{2!} u''(t) - \frac{\Delta t^3}{3!} u'''(t) + \frac{\Delta t^4}{4!} u''''(\eta)$$

we obtain

$$u''(t) \approx \frac{u(t + \Delta t) - 2u(t) + u(t - \Delta t)}{\Delta t^2}$$

We now use this approximation in our ODE to get a difference equation. If $U^k \approx u(t^k)$ then using the initial conditions $U^0 = 0$ and $u'(0) = 1$ implies $(U^1 - U_0)/\Delta t = 1$. Thus $U^1 = \Delta t + U^0$ and if $\Delta t = 0.1$, $U^1 = 0.1$; recall exact solution at 0.1 is $(.1)^4/12 + .1 = 1.001$ Then at $t = 2\Delta t$

$$\frac{U^2 - 2U^1 + U^0}{\Delta t^2} = (t^1)^2 = (\Delta t)^2 = 0.01 \Rightarrow U^2 = 0.2001$$

and the exact solution is 0.200133

Now let's change the problem in what appears on the surface to be a minor change but which, in fact, makes a huge change.

Example

$$-u''(x) = x \quad 0 < x < 2 \qquad u(0) = 0 \quad u(2) = 0$$

In this problem we know how u behaves at the endpoints of an interval and we want to find how it behaves in the interior.

- How does this compare with our previous problem?
- We call this problem a Boundary Value Problem (BVP).
- Can we use the same technique as above to solve it?

  Let $U_i \approx x_i$. Then $U^0 = 0$ and using the difference quotient

$$\frac{U_2 - 2U - 1 + U_0}{\Delta t^2} = x_1$$

Note that in this equation both U_2 and U_1 are unknowns whereas in the previous example, only U_2 was unknown. Consequently, we can't solve for U_2. The next equation gives a similar situation

$$\frac{U_3 - 2U - 2 + U_1}{\Delta t^2} = x_2$$

Here all three variables are unknown. The unknowns are all coupled together. This makes sense because we know that the right endpoint should also influence the solution, not just the left endpoint.

- How can we solve this linear algebraic system of equations?

  We write them as a matrix equation. For example, for five intervals

$$\begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{pmatrix} = \begin{pmatrix} \Delta x \\ 2\Delta x \\ 3\Delta x \\ 4\Delta x \end{pmatrix}$$

- Does this problem have a unique solution, i.e., is the coefficient matrix invertible?
- If the original ODE has a unique solution will the discrete problem also have a unique solution?
- We need to determine an efficient method for solving this linear system.
- There is not ONE method but rather many methods which fall into general class of direct or iterative methods.
- In direct methods we find the exact solution (if there was no roundoff) in a finite number of steps.
- In an iterative method, we start with an initial guess and generate a sequence of vectors which we hope converge to the exact solution; i.e., we can get as close as we want to the solution by taking more terms in the sequence.
- To choose the appropriate algorithm, you need to know the properties of the coefficient matrix - sparsity, symmetry, positive definiteness, etc.

  Now let's make another change to our problem and see it's effect.

Example

$$-u''(x) + u^2 = x \quad 0 < x < 2 \qquad u(0) = 0 \quad u(2) = 0$$

Again $U_0 = 0$ but now when we write the difference equation at dx we get

$$\frac{U_2 - 2U_1 + U_0}{\Delta t^2} + (U_1)^2 = x_1$$

and in general

$$\frac{U_{i+1} - 2U_i + U_{i-1}}{\Delta t^2} + (U_i)^2 = x_i$$

The problem is that we can no longer write our difference equations as a linear system because they are *nonlinear* due to the fact that the original ODE is nonlinear.

- We need to be able to recognize nonlinear ODEs and ultimately be able to approximate their solution.

Lastly, we ask ourselves what happens if the unknown u is a function of two independent variables instead of just one. Typically, we have either of the two situations illustrated below.

Example For a BVP where $u = u(x, y)$ we could have

$$-(u_{xx} + u_{yy}) = f(x, y) \quad 0 < x < 1, 0 < y < 1$$

$$u(0, y) = u(1, y) = 0 \qquad u(x, 0) = 2 \quad u(x, 1) = 1$$

Here the notation u_{xx} means the second partial of u with respect to x. We need to make sure that we understand what derivatives of functions of more than one variable means.

We can also have an initial boundary value problem (IBVP)

Example Let $u = u(x, t)$

$$u_t - u_{xx} = f(x, t) \quad 0 < t \leq T, \quad 0 < x < 1$$

$$u(x, 0) = u_0 \qquad u(0, t) = 1 \quad u(1, t) = 0$$

We will see that our techniques for ODEs can be expanded to solve these equations.

- We need to look at partial derivatives, directional derivatives, vector calculus before we address PDEs

Topics
- Linear algebra
- ODEs
- Multivariable calculus
- PDEs

- Not only is linear algebra essential to so many problems but if you have a firm foundation then it will help you understand more complicated mathematical topics.
- We have seen that discretization of DEs can lead to solving linear systems $A\vec{x} = \vec{b}$ where A is an $n \times n$ matrix and $\vec{x}, \vec{b}$ are n-vectors so we begin by considering this central problem.
- One approach which works well in learning/reviewing concepts in linear algebra is to *visualize* in two or three dimensions, then abstract to n dimensions. When considering methods we want to be cognizant of their use in computations.

Geometry of Linear Equations

We first begin with an example.

Example

$$\begin{aligned} 2x + y &= 4 \\ 3x - y &= 1 \end{aligned}$$

whose exact solution is $(1, 2)$.

One way to solve this is to plot the lines $y = 2x - 4$ and $y = 3x - 1$ and see the point (x, y) where they intersect. In this way we are concentrating on equations, i.e., rows but we also want to think about columns. We can also consider the problem of finding (x, y) such that

$$x \begin{pmatrix} 2 \\ 3 \end{pmatrix} + y \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \end{pmatrix}$$

We say that we want to determine the linear combination of the vectors $(2, 3)$ and $(1, -1)$ which yield $(4, 1)$. Sketch this graphically.

- In $\mathbf{R}^3$ when we look at the intersection of the equations then we find the intersection of three planes. For the columns, we now look for a linear combination of the columns (which are vectors in $\mathbf{R}^3$) which yields the right hand side.
- In $\mathbf{R}^n$ each row represents a hyperplane and we want to find the intersection of all of them. Again for the columns, we look for a linear combination of the columns (which are vectors in $\mathbf{R}^n$) which yields the right hand side which is a vector in $\mathbf{R}^n$.

What happens when no solution is found?

Example

$$\begin{aligned} 2x + y &= 4 \\ x + y/2 &= 1 \end{aligned}$$

When we plot these two equations we find that the lines are parallel and hence there is no point of intersection. If we consider the column approach then we want (x, y) such that

$$x \begin{pmatrix} 2 \\ 1 \end{pmatrix} + y \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \end{pmatrix}$$

But the column vectors are on the same line and the right hand side vector is not on that line so there is no way to combine them and get the right hand side vector.

- What is the analogous situation in $\mathbf{R}^3$? Be careful, there are three cases in $\mathbf{R}^3$.

What happens if infinitely many solutions are found?

Example

$$\begin{aligned} 2x + y &= 4 \\ x + y/2 &= 2 \end{aligned}$$

When we plot these two equations we find that the lines are the same so every point is a point of intersection and there are infinitely many solutions. If we consider the column approach then we want (x, y) such that

$$x \begin{pmatrix} 2 \\ 1 \end{pmatrix} + y \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \end{pmatrix}$$

But the column vectors are on the same line but now the right hand side vector is also on that line so there is are infinitely many ways to combine them and get the right hand side vector.

- What is the analogous situation in $\mathbf{R}^3$? Be careful, there are two cases in $\mathbf{R}^3$.

Gauss Elimination - A systematic method for finding the unique solution to a system of linear equations

When you took algebra, you learned this technique which is illustrated in the following example.

Example

$$\begin{aligned} 2x + y + z &= 5 \\ 4x - 6y &= -2 \\ -2x + 7y + 2z &= 9 \end{aligned}$$

Recall that we first eliminate x terms from the second and third equations by multiplying the first equation by a constant and add to the respective equation.

$$\begin{aligned} 2x + y + z &= 5 & \qquad 2x + y + z &= 5 \\ 4x - 6y &= -2 & \Rightarrow\ 0 - 8y - 2z &= -12 \\ -2x + 7y + 2z &= 9 & 0 + 8y + 3z &= 14 \end{aligned}$$

We multiplied the first equation by -2 and added to the second; then we multiplied the first equation by -1 and added to the third.

Now we want to eliminate y from the last equation. To this end we multiply the SECOND equation by 1 and add to the third equation to get

$$\begin{aligned} 2x+y+z&=5 \\ 0-8y-2z&=-12 \\ 0+8y+3z&=14 \end{aligned} \qquad \Rightarrow \begin{aligned} 2x+y+z&=5 \\ 0-8y-2z&=-12 \\ z&=2 \end{aligned}$$

The third equation only contains one unknown, z, so we solve for that and then in the second equation the unknowns are y, z but now we know z so we solve for y. Finally we substitute the values for y, z into the first equation and solve for x arriving at $(1, 1, 2)$ as the solution. We call the coefficient of x in the first equation (i.e., 2) and the coefficient of y after x has been eliminated (i.e., -8) *pivots.* When the last equation contains only one variable, the next to last only two variables, etc. then the process to solve the system is called *backsolving.*

- When will this process fail? Is it only when the system fails to have a unique solution?

Example

$$\begin{aligned} 2x+y+z&=5 \\ 4x-6y&=-2 \\ -2x-3y&=-1 \end{aligned}$$

Clearly, the last two equations are essentially the same so we should have infinitely many solutions. Here's what happens with Gauss elimination.

$$\begin{aligned} 2x+y+z&=5 \\ 4x-6y&=-2 \\ -2x+7y+2z&=9 \end{aligned} \quad \Rightarrow \begin{aligned} 2x+y+z&=5 \\ 0-8y-2z&=-12 \\ 0+4y-z&=-6 \end{aligned} \quad \Rightarrow \begin{aligned} 2x+y+z&=5 \\ 0-8y-2z&=-12 \\ 0&=0 \end{aligned}$$

- Will it fail at other times?

Example

$$\begin{aligned} y+z&=3 \\ 4x=6y&=-2 \\ -2x+7y+2z&=9 \end{aligned}$$

The procedure, as we described it, fails because x does not appear in the first equation and so we can't use it to eliminate x from the second and third equations. Of course, we could simply reorder the equations.

- Is having a zero pivot the only time the method can fail if the system has a unique solution?

If exact arithmetic is used and no roundoff occurs then the answer is yes. But when we work on a computer we are using finite precision arithmetic; for example 1/3 will not be entered exactly. Consider the following example where we will only assume we can only use two significant digits, i.e., every number can be written as $\pm 0.d_1 d_2 \ 10^e$ in our solution algorithm.

Example

$$\frac{1}{1000}x + y = 1$$
$$x + y = 2$$

whose exact solution is $x = 1000/999, y = 998/999$. We have

$$\begin{aligned} 0.10\ 10^{-2}x + 0.10\ 10^{1}y &= 0.10\ 10^{1} \\ 0.1\ 10^{1}x + 0.10\ 10^{1}y &= 0.20\ 10^{1} \end{aligned} \Rightarrow \begin{aligned} 0.10\ 10^{-2}x + 0.10\ 10^{1}y &= 0.10\ 10^{1} \\ 0.10\ 10^{4}y &= 0.10\ 10^{4} \end{aligned} \Rightarrow y = 1, x = 0$$

where in exact arithmetic we had 1-1000=-999 and 2 -1000=-998 but these have each been rounded to 1000=0.10 10^4 in two digit arithmetic. The problem here is that the pivot 1/1000 is small compared with the other entries. If we interchange rows, then we don't have any problem.

Example In this example, we multiply the first equation in the last example by 10,000. Now the pivot is not small but we still have problems.

$$10x + 10,000y = 10,000$$
$$x + y = 2$$

whose exact solution is the same as before $x = 1000/999, y = 998/999$. We have

$$\begin{aligned} 10x + 10,000y &= 10,000 \\ x + y &= 2 \end{aligned} \Rightarrow \begin{aligned} 10x + 10,000y &= 10,000 \\ (1 - 1000)y &= 2 - 1000 \end{aligned}$$

Using two digit arithmetic we have $-1000y = -1000$ or $y = 1$. Now $10x - 10,000 = 10,000$ implies $x = 0$. In this problem the difficulty is caused by scaling.

- Consequently, when we develop our computational algorithm we need to take all of these things into account.

Example A standard example of a system that is "difficult" to solve is due to Hilbert. For four equations we have the system

$$\begin{aligned} x_1 + \frac{1}{2}x_2 + \frac{1}{3}x_3 + \frac{1}{4}x_4 &= b_1 \\ \frac{1}{2}x_1 + \frac{1}{3}x_2 + \frac{1}{4}x_3 + \frac{1}{5}x_4 &= b_2 \\ \frac{1}{3}x_1 + \frac{1}{4}x_2 + \frac{1}{5}x_3 + \frac{1}{6}x_4 &= b_3 \\ \frac{1}{4}x_1 + \frac{1}{5}x_2 + \frac{1}{6}x_3 + \frac{1}{7}x_4 &= b_4 \end{aligned}$$

What makes this system so difficult to solve? Small changes in the data (e.g., entering 1/3 not exactly) can cause large changes in the solution. We say the system is *ill-conditioned.*

- We will need to find a way to determine if a system is ill-conditioned.