CHEE 3602 – Topic 7:
Ordinary differential equations

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Theoretical principles

Differential equations

- A differential equation is just an expression of a derivative
- Consider the following example

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x)$$

- The goal is to find $y = g(x)$

One example

One common example is that of cellular growth rate:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \mu X$$

The number of new cells being generated at some time t will depend on the number of cells at time t.

Another example

Reaction rate laws are another example:

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = -k_1 C_A - k_3 C_A C_B$$

$$\frac{\mathrm{d}C_B}{\mathrm{d}t} = -k_2 C_B - k_3 C_A C_B$$

$$\frac{\mathrm{d}C_C}{\mathrm{d}t} = k_3 C_A C_B$$

There is data on how the concentrations are changing, but it may be necessary to calculated the actual concentrations as a function of time.

Consider

These types of problems might look familiar to the last topic…

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x)$$

$$y = \int f(x)\mathrm{dx}$$

Why not just use Simpson's rule and call it a day?

Extending topic 6

The methods covered in Topic 6 implicitly assumed separable differential equations:

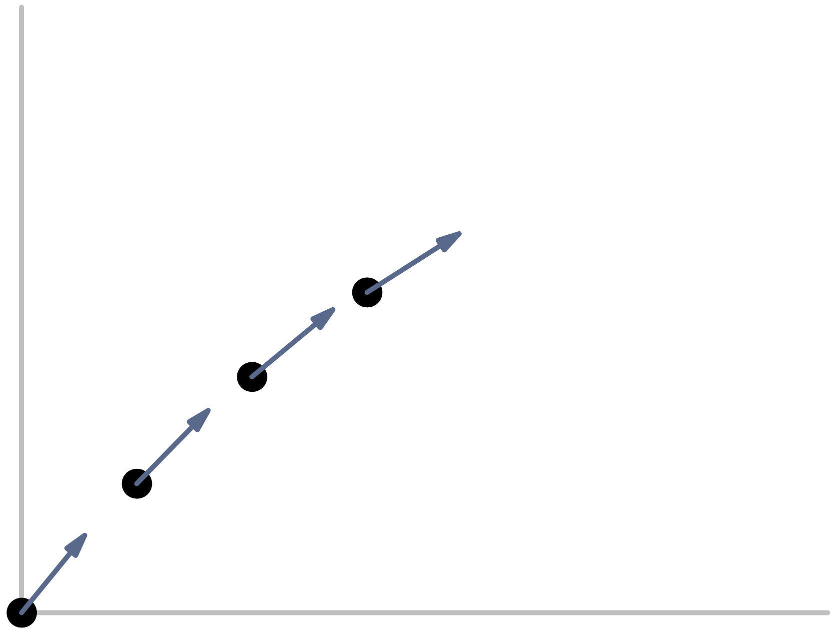
$$y = \int x \mathrm{dx}$$

But this is not the only type of differential equation... This topic introduces tools to solve a new class of problems:

$$y = \int x + y \mathrm{dx}$$

A new approach

Rather than taking an integral directly, all of the methods in this topic will rely on tracing y based on knowledge of how y is changing:



A new approach

Every technique that we will cover in this topic only differs by how the change is y is calculated.

Some nomenclature

It is important to understand how to classify differential equations — as different types of differential equations require different approaches.

Order

The order of a differential equation is the order of the highest differential.

First order example:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = x^2 + y$$

Second order example:

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = x^2 + y$$

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + \frac{\mathrm{d}y}{\mathrm{d}x} = x^2 + y$$

Variables

A dependent variable is one that is being differentiated with respect to the independent variable.

x is independent, y is dependent:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = x + y$$

x is independent, y and z are dependent:

$$\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\mathrm{d}z}{\mathrm{d}x} = x + y$$

x and y are independent, z is dependent:

$$\frac{\partial z}{\partial x} + \frac{\partial z}{\partial y} = x + y$$

Ordinary vs. partial differentials

An ordinary differential equation (ODE) contains differentials of variables with respect to only one independent variable. A partial differential equation (PDE) contains differentials with respect to multiple variables.

ODE:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = x + y$$

PDE:

$$\frac{\partial z}{\partial x} + \frac{\partial z}{\partial y} = x + y$$

Ordinary vs. partial differentials

Keep in mind that it is possible to have ODE equations with multiple dependent variables:

The following is still an ODE:

$$\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\mathrm{d}z}{\mathrm{d}x} = x + y$$

Often, a partial differential equations contains partial derivatives (∂x vs. $\mathrm{d}x$), but do not rely on everyone properly formatting their equation text.

An example from heat transfer

Example 1

List the dependent variables, independent variables, and constants in the following equations and classify the equations (based on the properties covered in class).

a) $\dfrac{\mathrm{d}T}{\mathrm{d}t} = -\dfrac{hA}{mc_p}(T - T_\infty)$

b) $\dfrac{\mathrm{d}T}{\mathrm{d}t} = \alpha\left(\dfrac{\partial^2 T}{\partial x^2} + \dfrac{\partial^2 T}{\partial y^2}\right)$

Heat and mass transfer

Heat and mass transfer is likely the biggest application of differential equations in chemical engineering. You will frequently see equations tracking temperature (T) or concentration (C) as a function of time (t) and spacial coordinates (x, y, z).

These equations will not go away so do your best to start remembering them!

Boundary information

- Indefinite integrals require the addition of a constant of integration
  - extra information is needed on top of the differential equation
- Typically, this information comes from boundary conditions
  - a first order differential equation requires one piece of information
  - the most common piece of information is the initial condition: y or $f(x, y)$ at $x = 0$
  - higher order equations require additional information

The initial value problem

- The following slides focus on solving just one type of ODE
  - first order initial value problem (IVP)
- This type of ODE is very common in chemical engineering
  - and will form the basis of more complex methods
- The same ideas can be applied to higher order problems

Standard notation

To solve differential equations using standard numerical methods, the equations must be arranged in standard notation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y)$$

For example:

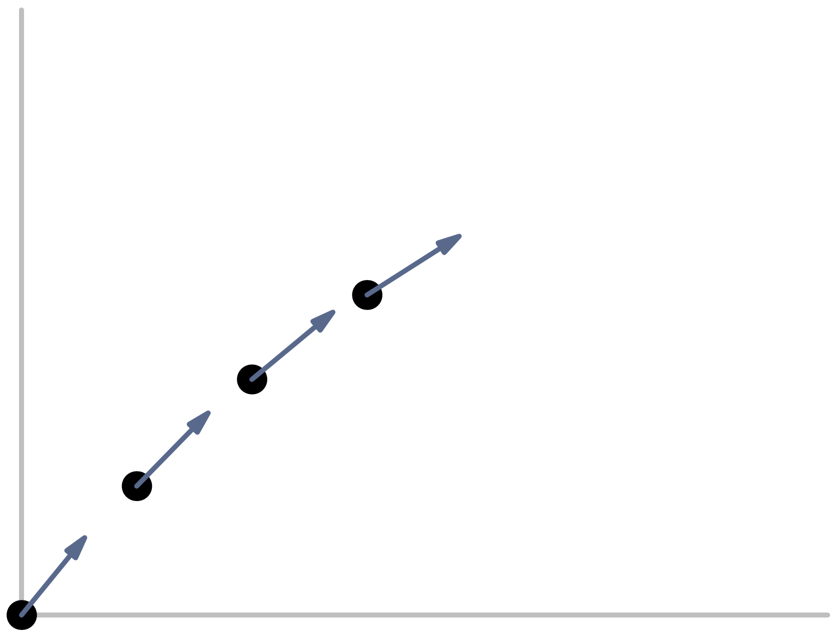
$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{1}{x + y + 1}$$

Each independent variable must be accompanied by a set of initial values:

$$y(x = 0) = 0$$

Standard notation

The overall strategy will be to calculate the rate of change at some initial point, use that rate of change to get the next point, and so on...



Systems of equations

Although the slides will focus on single equations for now, the exact same process can be applied to systems of equations:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y, z, z')$$
$$\frac{\mathrm{d}z}{\mathrm{d}x} = g(x, y, y', z)$$

For example:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{1}{x + y + 1} + \frac{\mathrm{d}z}{\mathrm{d}x}$$
$$\frac{\mathrm{d}z}{\mathrm{d}x} = \sin(x)$$

Systems of equations

Note that higher order ODEs can always be converted into a coupled system of lower order ODEs.

For example,

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + \frac{\mathrm{d}y}{\mathrm{d}x} = a$$

Can be transformed into:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = z$$

$$\frac{\mathrm{d}z}{\mathrm{d}x} = a - z$$