Week 10: PDE revision and the wave equation

Well posedness, stability and the CFL condition, the wave equation as an example

Dr K Clough, Topics in Scientific computing, Autumn term 2023

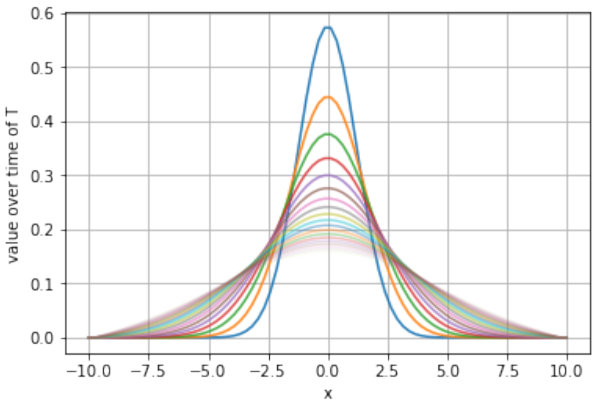
Plan for today

1. Revision of numerical differentiation
2. Revision of PDE types and their properties
3. Problems with PDEs - well posedness
4. Problems with PDEs - Von Neumann stability and the CFL condition
5. Solving second order in time PDEs - solution of the wave equation

Application: solving the heat equation

- In the tutorial you will solve the heat equation using solve_ivp()

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$




```python
def calculate_dydt(self, t, current_state) :

    # Just for readability
    dTdt = np.zeros_like(current_state)

    # Now actually work out the time derivatives
    dTdt[:] =  self.alpha * np.dot(self.D2_matrix, current_state)

    # Zero the derivatives at the end for stability
    # (especially important in the pseudospectral method)
    dTdt[0] = 0.0
    dTdt[1] = 0.0
    dTdt[self.N_grid-1] = 0.0
    dTdt[self.N_grid-2] = 0.0

    return dTdt
```

Derivatives - stencil representation

We can see ***finite differencing*** as the convolution of a stencil with the current state vector.

$\Delta x = 0.5$

Position x	0	0.5	1	1.5	2	2.5
Temperature T	0	1	3	2	1	0

4	-8	4

Second derivative stencil

$$\approx \frac{g(x+\Delta x) - 2g(x) + g(x-\Delta x)}{\Delta x^2}$$

d2T/dx2			**-12**			

Derivatives - matrix representation

Here we are using the matrix representation to calculate the time derivative

Position x	0	0.5	1	1.5	2	2.5
Temperature T	0	1	3	2	1	0

D2Tdx2 **=** ***Matrix D^2*** ***T***

$$\begin{bmatrix} 2 \\ 3 \\ 1 \\ -2 \\ -2 \\ -2 \end{bmatrix} = \begin{bmatrix} X & X & & & & \\ X & X & X & & & \\ & X & X & X & & \\ & & X & X & X & \\ & & & X & X & X \\ & & & & X & X \end{bmatrix} \bullet \begin{bmatrix} 0 \\ 1 \\ 3 \\ 2 \\ 1 \\ 0 \end{bmatrix}$$

Application: solving the heat equation

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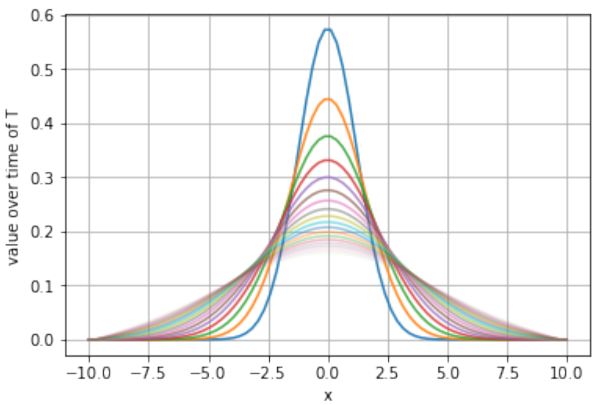


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Classification of second order PDEs

Consider the most general second order PDE for 1 dependent variable with 2 independent variables:

$$A\frac{\partial^2 u}{\partial x^2} + 2B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + F = 0$$

The equation is classified based on the discriminant $\Delta = B^2 - 4AC$:

$\Delta < 0$ Elliptic

$\Delta = 0$ Parabolic

$\Delta > 0$ Hyperbolic

Example 1: The heat equation

The heat equation, (α is a positive constant, S is any function of u, x and t but not their derivatives)

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + S$$

What type is this equation?

Example 1: The heat equation

The heat equation is a parabolic equation $\Delta = 0$

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + S$$

-> A = α, E = -1, B = C = D = 0, F = S

This equation is ***first order in time***, so solutions will evolve in time as exponentials in response to an instantaneous source. The dependence on the ***second derivative in space*** means that it has a tendency to smooth the solution - any bumps in the solution decrease in time.

The positive constant α controls the rate of diffusion of heat.

Example 1: The heat equation

The heat equation is a parabolic equation $\Delta = 0$

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + S$$

-> A = α, E = -1, B = C = D = 0, F = S

A typical solution has the form:

$$T(x,t) = Ae^{-t/\tau}e^{ikx} \sim Ae^{-t/\tau}\sin(kx)$$

(In general it will be a superposition of many such terms with different k)

Example 2: The wave equation

The wave equation (c is a positive constant, S is any function of u, x and t but not their derivatives)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} + S$$

What type is this equation?

Example 2: The wave equation

The wave equation is a hyperbolic equation $\Delta > 0$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} + S$$

-> A = c, C = -1, B = D = E = 0, F = S

This equation is ***second order in time***, so solutions will evolve in time with oscillations in response to an instantaneous source. The dependence on the ***second derivative in space*** means that it has a tendency to pull any bumps back towards zero displacement.

Hyperbolic equations have a finite speed of propagation of information - c.

Example 2: The wave equation

The wave equation is a hyperbolic equation $\Delta > 0$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} + S$$

-> A = c, C = -1, B = D = E = 0, F = S

A typical solution has the form:

$$T(x,t) = Ae^{i(wt-kx)} \sim A\cos(\omega t)\ \ \sin(kx)$$

(In general it will be a superposition of many such terms with different k)

Example 3: Poisson's equation

The Poisson equation (f is any function of u, x and t but not their derivatives)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

What type is this equation?

Example 3: Poisson's equation

The Poisson equation is an elliptic equation $\Delta < 0$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

-> A = 1, C = 1, B = D = E = 0, F = -f

This equation is ***second order in both dimensions, which are usually thought of as two spatial directions*** (for reasons we will discuss next). If the source f is zero it is called Laplace's equation, and for zero boundary conditions the solution is a constant. A non zero source creates a displacement or bump in the solution.

Elliptic equations have an infinite speed of propagation of information.

Example 3: Poisson's equation in 1D

The Poisson equation (f is any function of u, x and t but not their derivatives)

$$\frac{\partial^2 u}{\partial x^2} = f$$

What type is this equation?

Example 4: Poisson's equation in 1D

The Poisson equation (f is any function of u, x and t but not their derivatives)

$$\frac{d^2u}{dx^2} = f$$

Trick question! This is just an ODE like we studied before as there is only one independent variable!

Example 5: Katy's equation

Katy's equation (f is any function of u, x and t but not their derivatives)

$$\frac{\partial^2 u}{\partial t^2} + (t - 10)\frac{\partial^2 u}{\partial y^2} = f$$

What type is this equation?

Example 5: Katy’s equation

Katy’s equation (f is any function of u, x and t but not their derivatives)

$$\frac{\partial^2 u}{\partial t^2} + (t - 10)\frac{\partial^2 u}{\partial y^2} = f$$

This equation changes character at t=10 - before it is hyperbolic and after it is elliptic.

A system of PDEs can be of mixed type (e.g. Navier Stokes is mixed parabolic/hyperbolic) and they can change type at different points in space and time.

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Well posed problems - very active area of QMUL research!

- QMUL Maths is one of the leading places for solving issues of well-posedness.
- e.g. Prof Claudia Garetto of geometry, analysis and gravitation centre

On the well-posedness of weakly hyperbolic equations with time-dependent coefficients

Claudia Garetto [1], Michael Ruzhansky [2]

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Abstract

In this paper we analyse the Gevrey well-posedness of the Cauchy problem for weakly hyperbolic equations of general form with time-dependent coefficients. The results involve the order of lower order terms and the number of multiple roots. We also derive the corresponding well-posedness results in the space of Gevrey Beurling ultradistributions.

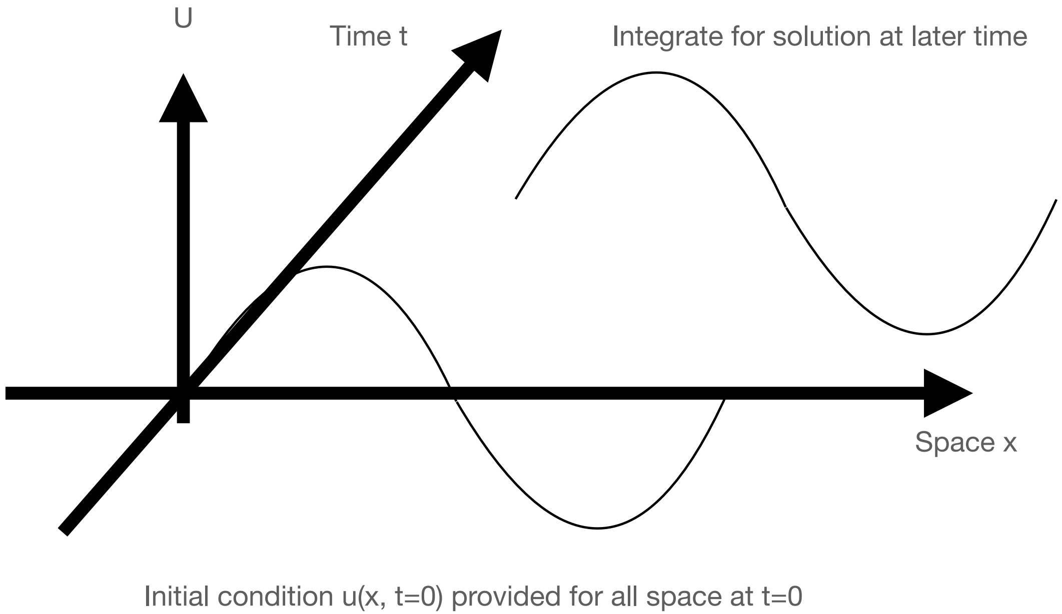
Well posed problems

- An initial value / Cauchy problem is well posed if:
  - A solution exists
  - The solution is unique
  - The solution depends continuously on the initial data

What is an initial value problem/Cauchy problem?

Initial value problem

- One of the independent variables is thought of as “time” (doesn’t have to actually ***be*** time)
- Boundary value is provided as a value of the function at some (arbitrary) time t=0
- Full solution is found by integrating in time
- We will see an alternative (boundary value solution via relaxation) next week



Well posed problems

- An initial value / Cauchy problem is well posed if:
  - A solution exists
  - The solution is unique
  - The solution depends continuously on the initial data

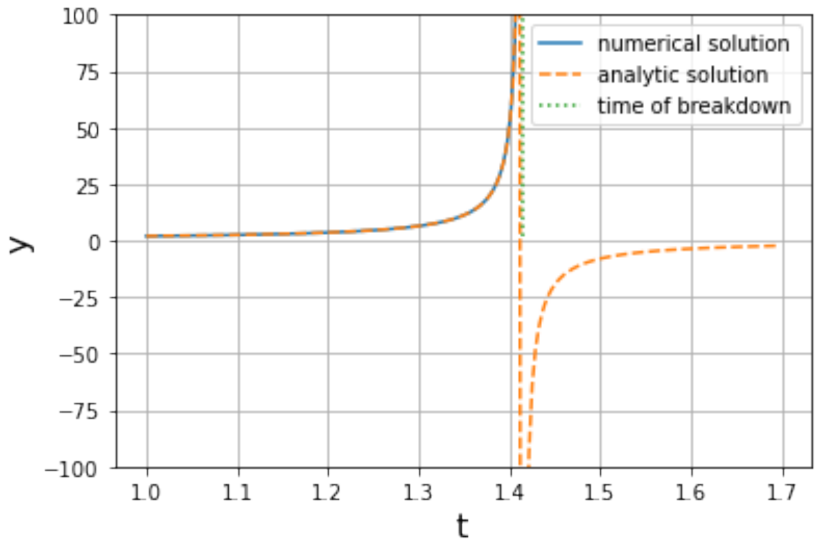
What did it mean for the solution to depend continuously on the initial data?

Well posed problems

Recall for ODEs:

- If $x_1(0) = a, x_2(0) = a + \delta$ it tells us that the solution changes by an amount that is bounded by $\delta\ e^{Lt}$ where L is some constant value - this is the meaning of "***depends continuously on the initial data***".

- We had the example that blows up at a value that depends on the initial conditions, so that a small change results in a change that is not bounded by an exponential



Well posed problems

- An initial value / Cauchy problem is well posed if:
  - A solution exists
  - The solution is unique
  - The solution depends continuously on the initial data

How can a solution not exist?

Well posed problems

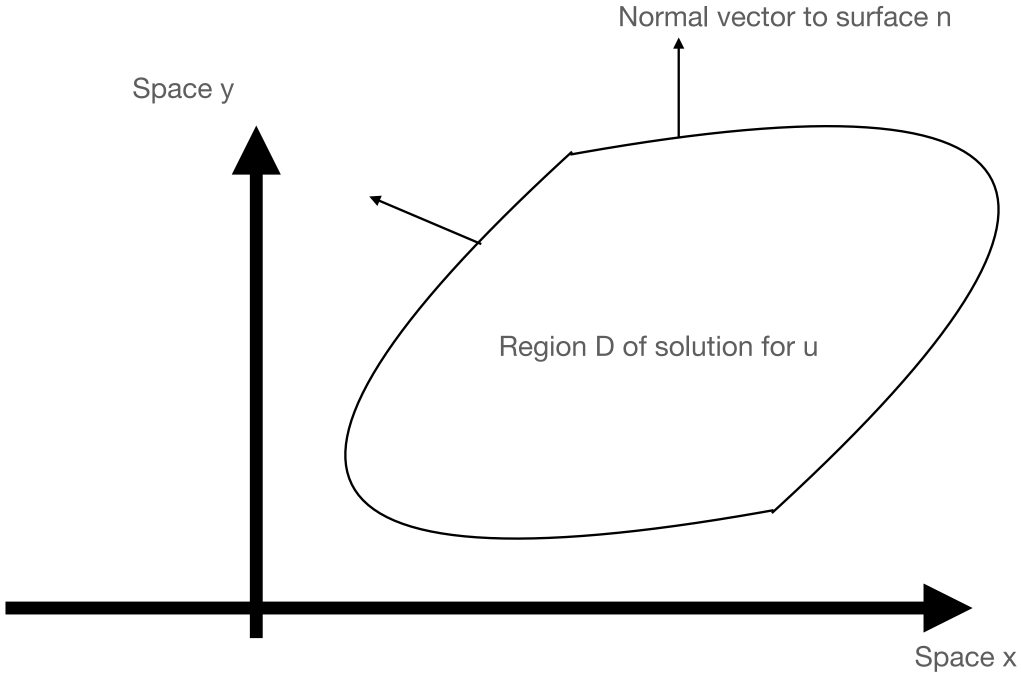
For Laplace's equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

with fixed boundary conditions

$$\nabla u \,.\, n = g(x, y) \quad (x, y) \in \partial D$$

No solution exists if $\displaystyle\int_{\partial D} g(x, y)\ ds \neq 0$



A nice detailed explanation is here: https://youtu.be/BmTFbUAOeec?si=22bdWktp55xLcT3s

Well posed problems

- An initial value / Cauchy problem is well posed if:
  - A solution exists
  - The solution is unique
  - The solution depends continuously on the initial data

How can a solution not be unique?

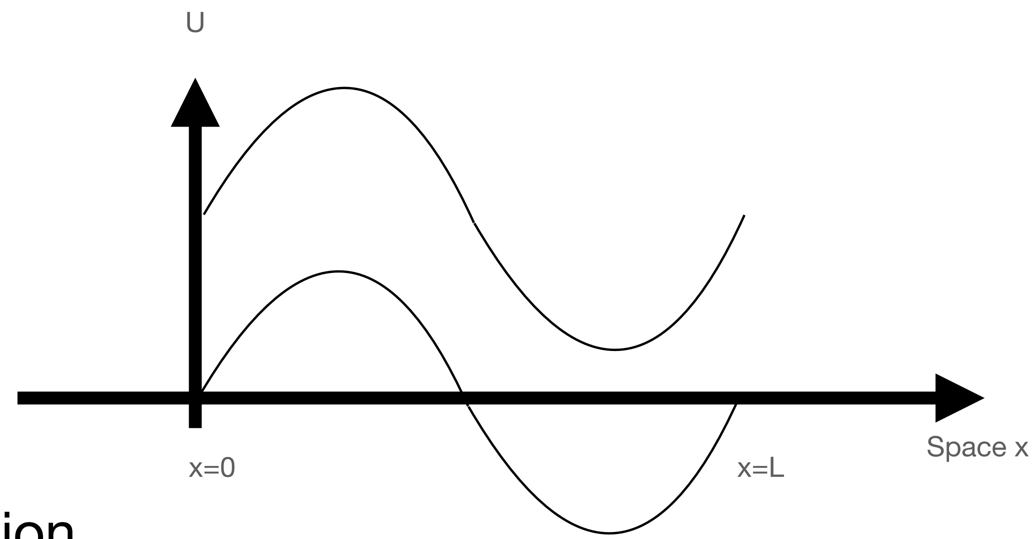
Well posed problems

Consider Poisson's equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

with periodic boundary conditions
$u(x = L) = u(x = 0)$

Then for any solution $u(x, t)$ the solution $\bar{u}(x, t) = u(x, t) + C$ with C a constant is also a solution.



Well posed problems

- Theorems in mathematics guarantee the (local) well-posedness of linear and quasi-linear* strongly hyperbolic* and parabolic PDEs.
- Elliptic PDEs do not admit a well-posed IVP. This does not (necessarily) mean they cannot be solved, just that another method may be required.
- When in a correct numerical implementation one increases the resolution and the solution blows up faster, that usually implies an ill-posed initial value problem.

*We will discuss the exact meaning of these terms next week.
For now just think of hyperbolic and parabolic equations as generally ok.

Well posed problems - why elliptic equations fail as an initial value problem

Consider Laplace's equation but treat one of the directions as a "time":

$$\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial x^2} = 0$$

And propose a wave like solution

$$u(x, t) = \exp(i[\omega t - kx])$$

Then

$$-\omega^2 u - k^2 u = 0 \quad \implies \omega = \pm\, i\,|\,k\,| \quad \implies u(x, t) = A \;\; \exp(\,|\,k\,|\,t + ikx) + \ldots$$

Which blows up exponentially at a faster rate for higher k (= shorter wavelengths)

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Von Neumann stability analysis and the CFL condition (Courant Friedrich Lewy)

- Like for ODEs, numerical schemes for PDEs can be unstable, and they have to be analysed for each PDE and PDE scheme separately

- For an initial value problem, this usually results in a “**CFL condition**” on the time step of the form:

$$\Delta t = \lambda \Delta x \qquad \text{for hyperbolic equations}$$
$$\Delta t = \lambda \Delta x^2 \qquad \text{for parabolic equations}$$

- The main method to determine the CFL number λ is called the Von Neumann stability analysis. It is a is ***necessary but not sufficient*** condition for stability.

Von Neumann stability analysis and the CFL condition

Method:

1. Calculate for the given numerical scheme the amplification factor between timesteps - assume that this is the same for the solution and the error

$$\Lambda = \frac{u_i^{n+1}}{u_i^n}$$

2. Make an assumption about the form of the solution

3. Require $|\Lambda| \leq 1$ for the solution error to not be amplified, which gives rise to a condition on Δt in terms of Δx.

Von Neumann stability analysis

e.g. Euler update for the heat equation, using 3 point stencil
(will do in lecture, but not examinable):

1. Calculate for the given numerical scheme the amplification factor between timesteps

$$T_i^{n+1} = T_i^n + \Delta t \ \frac{\partial T_i^n}{\partial t}$$

$$\implies T_i^{n+1} = T_i^n + \alpha \Delta t \ \frac{\partial^2 T_i^n}{\partial x^2}$$

$$\implies T_i^{n+1} \approx T_i^n + \alpha \frac{\Delta t}{(\Delta x)^2} (T_{i-1}^n - 2T_i^n + T_{i+1}^n)$$

Von Neumann stability analysis

e.g. Euler update for the heat equation, using 3 point stencil (will do in lecture, but not examinable):

2. Assume the form of solution for the heat equation

$$T(t, x) = E_k(t)e^{ikx}$$

$$\implies E_i^{n+1}e^{ikx} \approx E_i^n e^{ikx}\left[1 + \alpha\frac{\Delta t}{(\Delta x)^2}\left(e^{-ik\Delta x} - 2 + e^{ik\Delta x}\right)\right]$$

$$\implies E_i^{n+1}e^{ikx} \approx E_i^n e^{ikx}\left[1 - 4\alpha\frac{\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right]$$

Von Neumann stability analysis

e.g. Euler update for the heat equation, using 3 point stencil (will do in lecture, but not examinable):

3. The amplification factor should have a magnitude of less than 1

$$\implies E_i^{n+1} = E_i^n \left[1 - 4\alpha \frac{\Delta t}{(\Delta x)^2} \sin^2\left(\frac{k\Delta x}{2}\right)\right]$$

$$\implies \Lambda_{min} = \left|1 - 4\alpha \frac{\Delta t}{(\Delta x)^2}\right| \leq 1$$

$$\implies \Delta t \leq \frac{1}{2\alpha}(\Delta x)^2$$ CFL number is $\frac{1}{2\alpha}$

Von Neumann stability analysis and the CFL condition (Courant Friedrich Lewy)

- "**CFL condition**" on the time step of the form:

$$\Delta t = \lambda \Delta x \qquad \text{for hyperbolic equations}$$
$$\Delta t = \lambda \Delta x^2 \qquad \text{for parabolic equations}$$

- By physical arguments, we should expect $\lambda \leq 1/c$ (wave eqn) or $\lambda \leq 1/\alpha$ (heat eqn) since these constants determine the speed of propagation (if we take too big timesteps we don't respect causality).

- In practise - we can usually just use trial and error to find how high/low λ can be before the code becomes numerically unstable.

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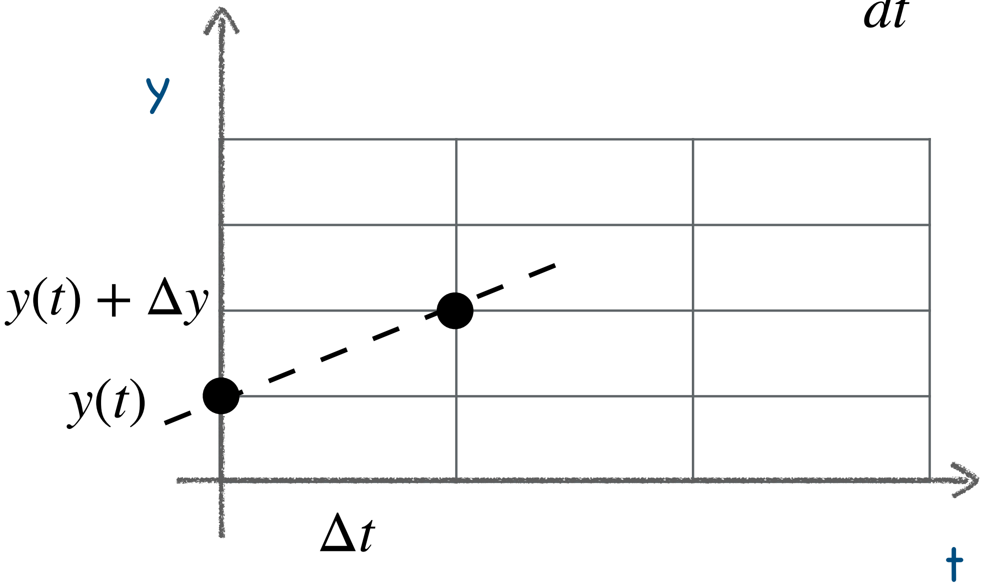
Recall: How do I integrate second order ODEs numerically?

$$\frac{d^2y}{dt^2} - \frac{dy}{dt} + f(y,t) = 0$$

$$\begin{cases} \dfrac{dv}{dt} - v + f(y,t) = 0 \\ \dfrac{dy}{dt} = v \end{cases}$$

1. Decompose the second order equation into two first order ones



$$\Delta v = \Delta t \left(v - f(y,t) \right)$$

$$\Delta y = v \ \Delta t$$

2. Solve as a dimension 2 first order system

Solving second order PDEs - the wave equation

Consider the wave equation for u:

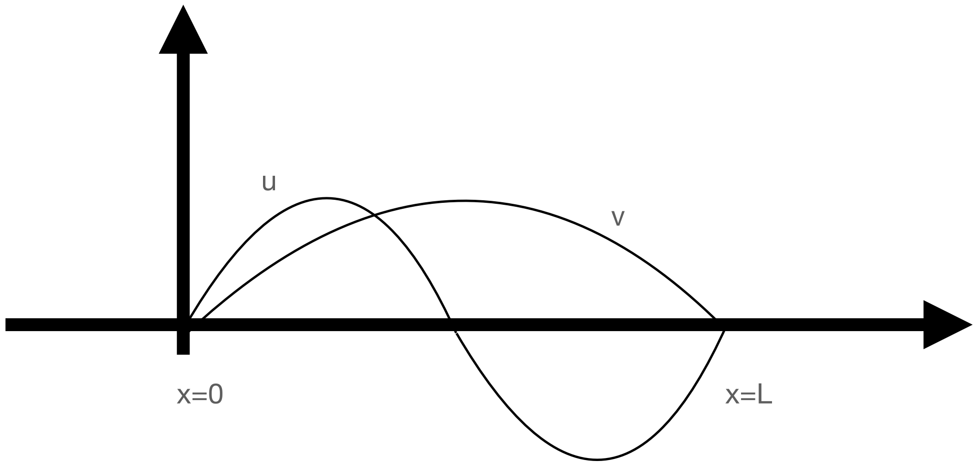
$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

And define the time derivative to be

$$v(x,t) = \frac{\partial u}{\partial t}$$

Then we solve the coupled system:

$$\frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad \frac{\partial u}{\partial t} = v$$



Wave equation - matrix representation

Recall that we can also represent this in matrix form: $\frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ $\frac{\partial u}{\partial t} = v$

dv/dt		***Matrix D^2***							***u***
2	=	X	x					•	0
3		1	-2	1					1
1	=		1	-2	1				3
-2				1	-2	1			2
-2					1	-2	1		1
-2						x	x		0

All blank entries zero

Wave equation - matrix representation

Recall that we can also represent this in matrix form: $\frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ $\frac{\partial u}{\partial t} = v$

$$
\underset{\textbf{du/dt}}{\begin{bmatrix} 2 \\ 3 \\ 1 \\ -2 \\ -2 \\ -2 \end{bmatrix}}
=
\underset{\textbf{Matrix I}}{\begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{bmatrix}}
\bullet
\underset{\textbf{v}}{\begin{bmatrix} 0 \\ 1 \\ 3 \\ 2 \\ 1 \\ 0 \end{bmatrix}}
$$

All blank entries zero

Wave equation - state vector in python

Need to unpack and repack the state vector in python.

Some useful commands:

```
u0 = get_y_test_function(x_values)
v0 = np.zeros_like(u0)
y0 = np.concatenate([u0,v0])
```

```
# Just for readability
[u,v] = np.array_split(current_state, 2)
dydt = np.zeros_like(current_state)
dudt, dvdt = np.array_split(dydt, 2)
```

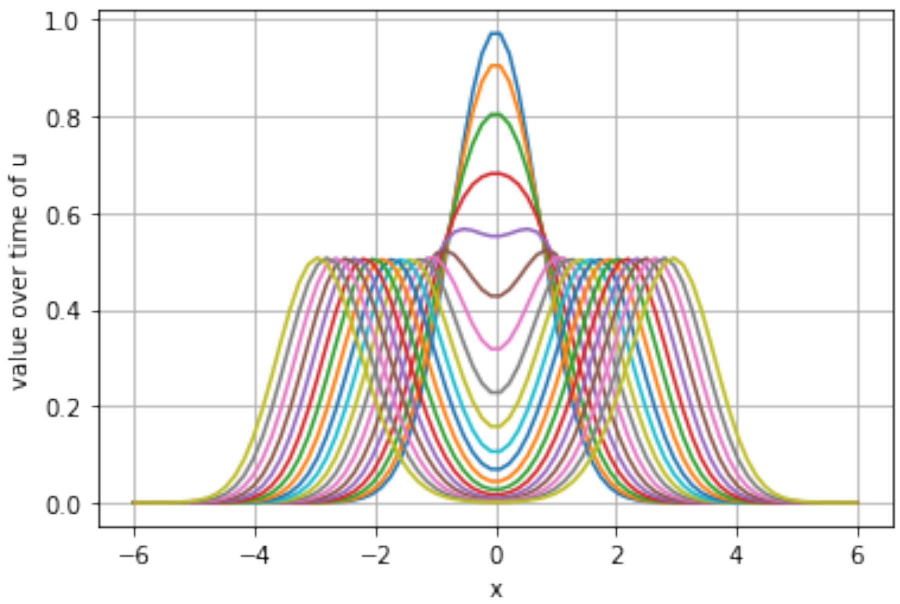
```
dudt[:] =  v
```

y

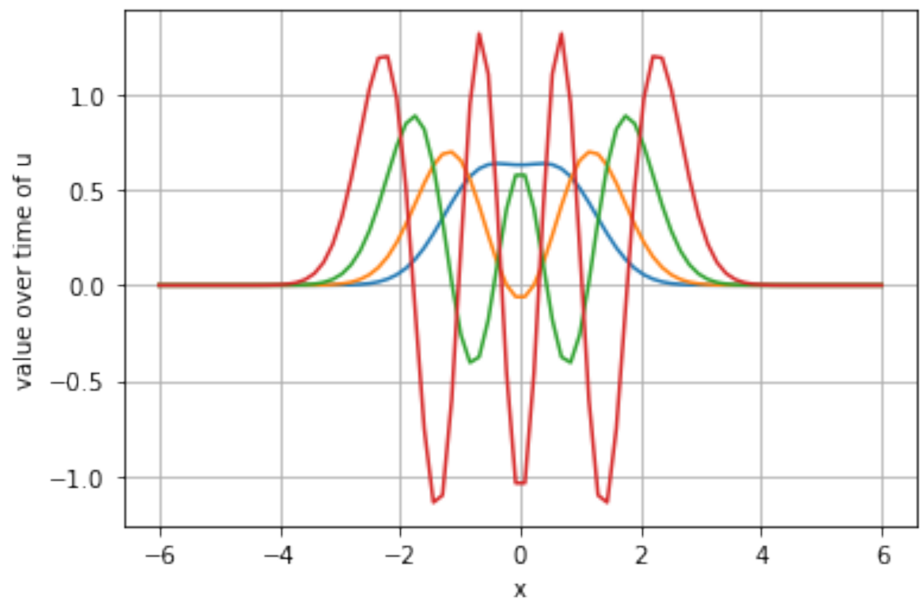
	2
	3
	1
u	-2
	-2
	-2
	0
	1
v	3
	2
	1
	0

Wave equation - tutorial

In the tutorial you will update the heat equation code from last week for the wave equation, and test the CFL condition.



CFL condition respected



CFL condition not respected

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