Math 260: Python programming in math

Fall 2020

Finite differences:
Boundary value problems and PDEs

Finite differences

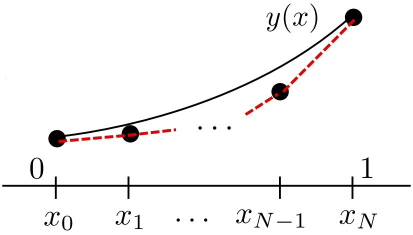
Here's an example of a linear algebra problem (with some ODE context)...

Suppose we want to solve, for $y(x)$, the **boundary value problem**

$$y'' - y = x, \qquad y(0) = 1,\ y(1) = e - 1$$

which has the solution $y(x) = e^x - x$.
Unlike an initial value problem, we can't just 'start' at an endpoint!

An approach is to approximate the function at mesh points x_j...



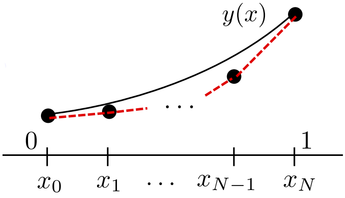
...and use the approximation

$$y''(x) \approx \frac{y(x+h) - 2y(x) + y(x-h)}{h^2}$$

for the second derivative.

Finite differences

$$y'' - y = x,$$
$$y(0) = 1,\ y(1) = e - 1$$



Let $x_j = jh$ be the mesh points ($h = 1/N$). Then, at x_j,

$$\frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} - y_j \approx x_j$$

The formula for our approximation u_j is then

$$u_{j+1} - 2u_j + u_{j-1} - h^2 u_j = h^2 x_j, \quad j = 1, \cdots, N-1$$

for the 'interior' points.
At the endpoints, we impose **boundary conditions**

$$u_0 = 1, \quad u_N = e - 1$$

Finite differences

To summarize, we have the problem/appproximation

$$y'' - y = x,$$
$$y(0) = 1,\ y(1) = e - 1$$

For $j = 1, 2, \cdots, N-1$,

$$u_{j+1} - (2 + h^2)u_j + u_{j-1} = h^2 x_j$$
$$u_0 = 1, \quad u_N = e - 1$$

Example: With five mesh points $0, 0.25, \cdots, 1$ we have $h = 0.25$ and

$$u_2 - (2 + h^2)u_1 + 1 = h^2 x_1$$
$$u_3 - (2 + h^2)u_2 + u_1 = h^2 x_2$$
$$e - 1 - (2 + h^2)u_3 + u_2 = h^2 x_3$$

which is the linear system

$$\begin{bmatrix} 2+h^2 & -1 & 0 \\ -1 & 2+h^2 & -1 \\ 0 & -1 & 2+h^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = -h^2 \begin{bmatrix} 0.25 \\ 0.5 \\ 0.75 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ (e-1) \end{bmatrix}$$

Finite differences

$$u_{j+1} - (2 + h^2)u_j + u_{j-1} = h^2 x_j, \quad j = 1, \cdots, N-1$$
$$u_0 = u_N = 0.$$

In general, the system to solve has the form

$$\begin{bmatrix} 2+h^2 & -1 & 0 & \cdots & 0 \\ -1 & 2+h^2 & -1 & \ddots & \vdots \\ 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2+h^2 & -1 \\ 0 & \cdots & 0 & -1 & 2+h^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = -h^2 \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-2} \\ x_{N-1} \end{bmatrix} - \begin{bmatrix} u_0 \\ 0 \\ \vdots \\ 0 \\ u_N \end{bmatrix}$$

- The matrix has three diagonals (around the center), called **tri-diagonal**
- Matrices like this how up often when data relates only to adjacent data
- We can solve using Gaussian elimination!

But GE takes $O(n^3)$ work... but only $\approx 3n$ non-zeros - can we do better?

Finite differences

The answer is yes - we can get $O(n)$ time - extremely fast!

Now forget about the ODE context and just consider trying to solve

$$A\mathbf{x} = \mathbf{b}, \qquad A = \begin{bmatrix} q_1 & r_1 & 0 & \cdots & 0 \\ p_2 & q_2 & r_2 & \ddots & \vdots \\ 0 & p_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & q_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & p_n & q_n \end{bmatrix}$$

Let's first look at an example, where we use GE to reduce

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

and get the LU factorization ($A = LU$).

Finite differences

Here entries of L are noted in red (in the zeroed entries).

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \Longrightarrow A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -0.5 & 1.5 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

(Zero out $(2, 1)$ entry using $R_2 \leftarrow R_2 + 0.5R_1$).
From here, we use 'lazy' notation: X denotes a value we *could* compute.

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -0.5 & 1.5 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \Longrightarrow \begin{bmatrix} 2 & -1 & 0 & 0 \\ -0.5 & 1.5 & -1 & 0 \\ 0 & X & X & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

(Zero out $(3, 2)$ entry using $R_3 \leftarrow R_3 + (1/2.5)R_2$.

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -0.5 & 1.5 & -1 & 0 \\ 0 & X & X & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \Longrightarrow \begin{bmatrix} 2 & -1 & 0 & 0 \\ -0.5 & 1.5 & -1 & 0 \\ 0 & X & X & -1 \\ 0 & 0 & X & X \end{bmatrix}$$

Done! Notice the mostly-zero structure has greatly simplified things...

Tridiagonal matrices

Thus we have found that the result looks like (X being some numbers)

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix} \Longrightarrow \begin{bmatrix} 2 & -1 & 0 & 0 \\ X & X & -1 & 0 \\ 0 & X & X & -1 \\ 0 & 0 & X & X \end{bmatrix}$$

$$\Longrightarrow A = LU \text{ where } L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ X & 1 & 0 & 0 \\ 0 & X & 1 & 0 \\ 0 & 0 & X & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 2 & -1 & 0 & 0 \\ 0 & X & -1 & 0 \\ 0 & 0 & X & -1 \\ 0 & 0 & 0 & X \end{bmatrix}$$

This process generalizes to the $N \times n$ tri-diagonal matrix, where:

- We only need to zero out one entry below the diagonal for each column
- The upper-diagonal never changes
- Both L and U have one diagonal other than the center ('bi-diagonal')

Tridiagonal matrices

Now let's derive an efficient Gaussian elimination for a tridiagonal matrix:

$$\begin{bmatrix} q_1 & r_1 & 0 & \cdots & 0 \\ p_2 & q_2 & r_2 & \ddots & \vdots \\ 0 & p_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & q_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & p_n & q_n \end{bmatrix} \implies \begin{bmatrix} d_1 & r_1 & 0 & \cdots & 0 \\ \ell_2 & d_2 & r_2 & \ddots & \vdots \\ 0 & \ell_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & d_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & \ell_n & d_n \end{bmatrix}$$

We want to find the ℓ's and d's.
First, $d_1 = q_1$ trivially. Then the first step of GE gives

$$\ell_2 = \frac{p_2}{d_1}, \quad d_2 = q_2 - \ell_2 r_1, \qquad \text{(multiplier: } \ell_2)$$

Then for the next step after that (and so on),

$$\ell_3 = \frac{p_3}{d_2}, \quad d_3 = q_3 - \ell_3 r_2,$$

$$\ell_j = \frac{p_j}{d_{j-1}}, \quad d_j = q_j - \ell_j r_{j-1}, \quad j = 2, 3 \cdots, n.$$

Thus we can solve for variables in the order

$$\ell_2 \to d_2 \ \to \ \ell_3 \to d_3 \ \to \cdots \ell_n \to d_n.$$

Tridiagonal matrices

Finally, to solve $Ax = b$ we solve

$$Ly = b, \qquad Ux = y.$$

Both solves are quite fast - forward/back substitution also simplify!

Forward solve: we have

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ \ell_2 & 1 & \ddots & \vdots \\ \vdots & \ddots & 1 & 0 \\ 0 & \cdots & \ell_n & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \implies y_j + \ell_j y_{j-1} = b_j$$

so y is given by

$$y_1 = b_1, \quad y_j = b_j - \ell_j y_{j-1}, \quad j = 2, \cdots, n.$$

Tridiagonal matrices

Finally, to solve $Ax = b$ we solve

$$Ly = b, \qquad Ux = y.$$

Both solves are quite fast - forward/back substitution also simplify!

Backward solve: Similarly,

$$\begin{bmatrix} d_1 & r_1 & \cdots & 0 \\ 0 & d_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & r_{n-1} \\ 0 & \cdots & 0 & d_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \implies d_j x_j + r_j x_{j+1} = y_j$$

so we can solve for $\mathbf{x}$ by

$$x_n = y_n / d_n, \quad x_j = \frac{y_j - r_j x_{j+1}}{d_j}, \quad j = n-1, n-2, \cdots, 1$$

Tridiagonal matrices

In summary, we have an efficient Gaussian elimination for solving $Ax = b$ where

$$A = \begin{bmatrix} q_1 & r_1 & 0 & \cdots & 0 \\ p_2 & q_2 & r_2 & \ddots & \vdots \\ 0 & p_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & q_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & p_n & q_n \end{bmatrix} \Longrightarrow \begin{bmatrix} d_1 & r_1 & 0 & \cdots & 0 \\ \ell_2 & d_2 & r_2 & \ddots & \vdots \\ 0 & \ell_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & d_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & \ell_n & d_n \end{bmatrix}$$

This method is sometimes called the **Thomas algorithm**.

- (**initialize**) Set $d_1 = q_1$ and $y_1 = b_1$.
- (**LU and fwd. solve**) Then for $j = 2, \cdots, n$:

$$\ell_j = p_j / d_{j-1}, \quad d_j = q_j - \ell_j r_{j-1}$$

$$y_j = b_j - \ell_j y_{j-1}.$$

- (**Back solve**) Finally set $x_n = y_n / d_n$ and for $j = n-1, n-2, \cdots, 1$:

$$x_j = (y_j - r_j x_{j+1}) / d_j.$$

Note that you can do the $Ux = y$ solve in parallel with the LU.

Tridiagonal matrices

A **tridiagonal matrix** should be stored in **banded form**:

$$A = \begin{bmatrix} q_1 & r_1 & 0 & \cdots & 0 \\ p_2 & q_2 & r_2 & \ddots & \vdots \\ 0 & p_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & q_{n-1} & r_{n-1} \\ 0 & \cdots & 0 & p_n & q_n \end{bmatrix} \text{ is stored as } \begin{bmatrix} 0 & q_1 & r_1 \\ p_2 & q_2 & r_2 \\ \vdots & \vdots & \vdots \\ p_{N-1} & q_{N-1} & r_{N-1} \\ p_{N-1} & q_{N-1} & 0 \end{bmatrix}$$

Pay attention to:

- The zeros - not part of the data (correct code should never read them!)
- Conventions may differ on the unused zeros (**'padding'**)
- Indexing (easy to be off by one!). Here:

$$\text{row } k \text{ of the array} \iff \text{row } k \text{ of the matrix}$$

We store only $3n$ numbers - much more feasible than n^2.

Code structure

See example code for the finite difference method. We solve

$$y'' - y = x, \quad y(0) = y_a, \quad y(b) = y_b$$

by solving the linear system In general, the system to solve has the form

$$\begin{bmatrix} 2+h^2 & -1 & 0 & \cdots & 0 \\ -1 & 2+h^2 & -1 & \ddots & \vdots \\ 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2+h^2 & -1 \\ 0 & \cdots & 0 & -1 & 2+h^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = -h^2 \begin{bmatrix} h^2 x_1 - y_a \\ h^2 x_2 \\ \vdots \\ h^2 x_{N-2} \\ h^2 x_{N-1} - y_b \end{bmatrix} \quad \text{(FD)}$$

breaking up into the following functions:

a) `build_fd` that creates A (as an array `bands`) and `rhs` as in (FD)

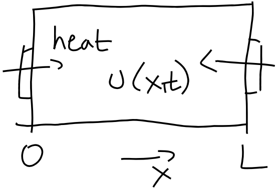
b) `trisolve(bands, rhs)`: solves $Ax = $ `rhs`, with A tri-diagonal

- A `solve` 'main' function that:
  - gets the $Ax =$ `rhs` system from (a)...
  - then solves it using (b).

From ODEs to partial differential equations...

PDEs and the method of lines

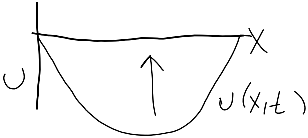
Suppose I am in a (cold) 1d room of length L.
I open windows at both ends to the outside.



Let the temperature in the room be $u(x,t)$.
Over time, u will equalize with the outside.

This process is modeled by the **heat equation**

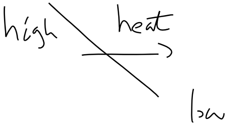
$$\frac{\partial u}{\partial t} = \beta \frac{\partial^2 u}{\partial x^2}$$



which is a **partial differential equation**
(it has derivs. in x **and** t).

Physical interpretation ('Fourier's law'):

$$\text{heat flow per time} = -\beta \frac{\partial u}{\partial x}.$$



That is, heat flows from *higher* to *lower*
temperature, and faster if the difference is large.

The heat equation

Other heat-like equations (different fluxes):

- Fisher's equation (genetics):

$$\frac{\partial f}{\partial t} = \frac{\partial^2}{\partial x^2}(x(1-x)f(x,t))$$

(describes distribution $f(x,t)$ of a trait in a population - "genetic drift")

- Black-Scholes - derivatives in finance
- Height of a liquid droplet $h(x,t)$ ("Porous medium equation")

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}(h^3\frac{\partial h}{\partial x})$$

- "advection-diffusion":

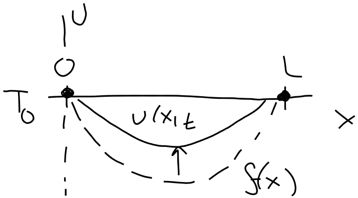
$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(F(u)) = \nu\frac{\partial^2 u}{\partial x^2}$$

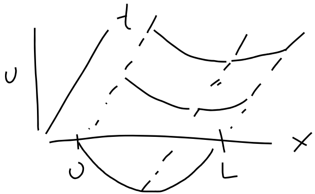
e.g. transport of a chemical in a solution

- And much more!

Can be solved with similar methods!

PDEs and the method of lines





$$\frac{\partial u}{\partial t} = \beta \frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \quad t > 0.$$

To complete the problem, there are also **initial conditions**

$$u(x, 0) = f(x) \text{ (initial distribution of heat)}$$

and **boundary conditions** (where T_0 is the outside temp.)

$$u(t, 0) = u(t, L) = T_0 \quad \text{for all } t.$$

The goal: reduce the problem into manageable pieces for computation.
We'll need: derivative approximations, an ODE solver, and a bit more.

Finite differences

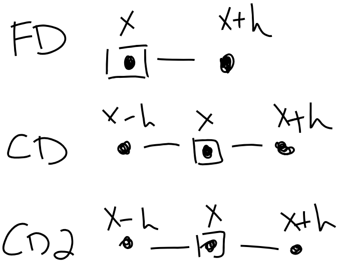
First, let's review some ways of approximating derivatives...

$$\text{Forward difference: } f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$\text{Central difference: } f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$\text{Central (2nd) difference: } f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

A 'stencil' diagram shows the points used in the approximation:



PDEs and the method of lines

We'll solve the heat equation using the **method of lines.**

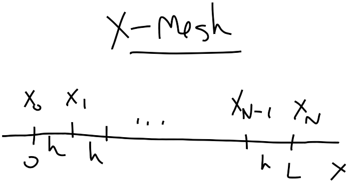
$$\frac{\partial u}{\partial t} = \beta \frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \quad t > 0.$$

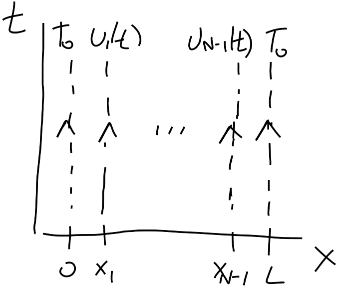
Step 1 (define a mesh in space): First define the points in *space* where the approximation is defined...

$$x_j = jh, \quad j = 0, 1, \cdots, N, \qquad \text{where } h = L/N.$$

Now think of u at each fixed x as a function in t:

$$u(x_j, t) := u_j(t) \text{ along the 'line' } x = x_j \;\; t > 0.$$





PDEs and the method of lines

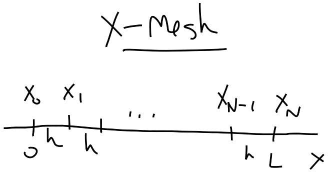
$$\frac{\partial u}{\partial t} = \beta \frac{\partial^2 u}{\partial x^2}, \qquad x \in (0, L), \quad t > 0.$$

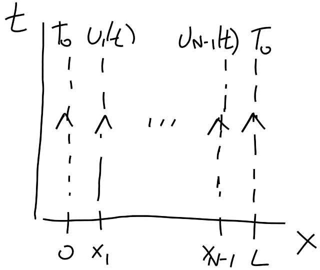
Step 2 (approximate x-derivatives): Using the central difference in x,

$$\frac{\partial u}{\partial t} \approx \beta \frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2}.$$

$$\text{At } x = x_j: \qquad \frac{du_j}{dt} \approx \beta \frac{u_{j+1} - u_j + u_{j-1}}{h^2}, \quad j = 1, \cdots, N-1$$

which is a system of **ODEs** for the functions along each 'line'.





The boundary conditions give the last two equations... $(u_0 = u_N = T_0)$.

PDEs and the method of lines

We have derived a system of $N-2$ ODEs

$$\frac{du_j}{dt} \approx \beta \frac{u_{j+1} - u_j + u_{j-1}}{h^2}, \quad j = 1, \cdots, N-1$$

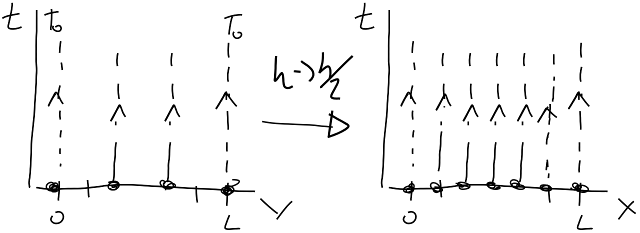
$$u(t,0) = u(t,L) = T_0 \implies u_0(t) = u_N(t) = T_0.$$

The initial conditions come from the IC for the original problem:

$$u(x,0) = f(x) \implies u_j(0) = f(x_j).$$

This system approximates the solution to the PDE (the **method of lines**).

As $h \to 0$ (i.e. as $N \to \infty$), it can be shown to converge.
(That is, a higher density of lines will give a better solution).



The ODE system can now be solved by any usual method. In summary:

$$\frac{du_j}{dt} \approx \beta \frac{u_{j+1} - u_j + u_{j-1}}{h^2}, \quad j = 1, \cdots, N-1$$

$$u(t,0) = u(t,L) = T_0 \implies u_0(t) = u_N(t) = T_0.$$

$$u_j(0) = f(x_j).$$

As an example, let's see what **Euler's method** looks like.

Our system is already in 'generic first order system form'

$$\mathbf{u}' = G(\mathbf{u}), \qquad \mathbf{u}(0) = (f(x_1), \cdots, f(x_{N-1}))$$

where $\mathbf{u}(t) = (u_1(t), \cdots, u_{N-1}(t))$ and G has components

$$G_j(\mathbf{u}) = \frac{\beta}{h^2}(u_{j+1} - 2u_j + u_{j-1}), \quad j = 1, \cdots, N-1$$

with u_0 and u_N replaced by T_0.

PDEs and the method of lines

For implementation, we just need to create the system of ODEs:

$$\mathbf{u}' = G(\mathbf{u}), \qquad \mathbf{u}(0) = (f(x_1), \cdots, f(x_{N-1}))$$

for $\mathbf{u} = (u_1, \cdots, u_{N-1})$ with

$$G_j(\mathbf{u}) = \frac{\beta}{h^2}(u_{j+1} - 2u_j + u_{j-1}), \quad j = 1, \cdots, N-1,$$

$$u_0(t) = u_N(t) = T_0.$$

Let's define $c = \beta/h^2$. A simple implementation:

```
def odefunc(t, u, c, ul, ur):
    n = len(u) + 2 # u = (u_1, ... u_(n-1))
    du = np.zeros(m)
    for j in range(1, n-2): # interior points
        du[j] = a*(u[j+1] - 2*u[j] + u[j-1])

    # boundary points
    du[0] = a*(u[1] - 2*u[0] + ul)       # x= 0
    du[n-2] = a*(ur - 2*u[n-2] + u[n-3]) # x = L
    return du
```

(Note: to improve this, have odefunc not create a new array each call).

PDEs and the method of lines

With $\mathbf{u}(t) = (u_1(t), \cdots, u_{N-1}(t))$,

$$\mathbf{u}' = G(\mathbf{u}), \qquad \mathbf{u}(0) = (f(x_1), \cdots, f(x_{N-1}))$$

$$G_j(\mathbf{u}) = \frac{\beta}{h^2}(u_{j+1} - 2u_j + u_{j-1}), \quad j = 1, \cdots, N-1$$

Let $\mathbf{u}^{(k)}$ denote the solution vector at time t_k.
We use a **super**-script for time,
and **sub**-script for space here, so

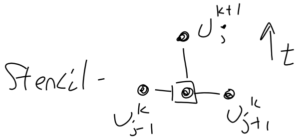
$$\mathbf{u}^{(k)} = (u_1(t_k), \cdots, u_{n-1}(t_k))$$

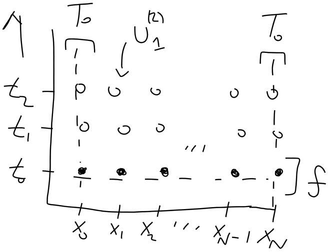
Euler's method approximates at times

$$0 = t_0 < t_1 < \cdots$$

where we assume that the t's have an equal spacing Δt. Then

$$\mathbf{u}^{(k+1)} = \mathbf{u}^k + \Delta t G(\mathbf{u}^k), \quad k = 0, 1, \cdots.$$





PDEs and the method of lines

Euler's method:

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{k} + \Delta t G(\mathbf{u}^{k}), \quad k = 0, 1, \cdots .$$

This is enough to write up the code, but it's worth 'plugging in' G,

$$G_j(\mathbf{u}) = \frac{\beta}{h^2}(u_{j+1} - 2u_j + u_{j-1}), \quad j = 1, \cdots, N-1.$$

For the j-th component,

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^k - 2u_j^k + u_{j-1}^k)$$

Set $a = \beta \Delta t / h^2$. This equation is **linear** in u. In matrix form...

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}^{(k+1)} = \begin{bmatrix} 1-2a & a & \cdots & 0 \\ a & 1-2a & \ddots & \vdots \\ \vdots & \ddots & \ddots & a \\ 0 & \cdots & a & 1-2a \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}^{(k)} + \begin{bmatrix} aT_0 \\ 0 \\ \vdots \\ 0 \\ aT_0 \end{bmatrix}$$

Note that $u_0(t) = u_N(t) = T_0$ has been plugged in here.

PDEs and the method of lines

Euler's method:

$$\mathbf{u}^{(k+1)} = \mathbf{u} + \Delta t G(\mathbf{u}^k), \quad k = 0, 1, \cdots .$$

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^k - 2u_j^k + u_{j-1}^k)$$

We can simplify a bit by defining the 'differentiation matrix'

$$D = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & \cdots & 0 \\ 1 & -2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \cdots & 1 & -2 \end{bmatrix}, \qquad (D\vec{f})_j \approx f''(x_j).$$

Then, from the previous slide, Euler's method becomes

$$\mathbf{u}^{(k+1)} = (I + \Delta t D)\mathbf{u}^{(k)} + \mathbf{b}$$

It's worth noting that:

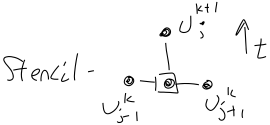
- This matrix form is nice for theory...
- ... but the ODE or difference formula are used in implementation

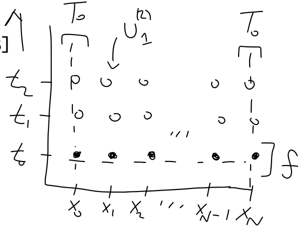
Euler's method (directly)

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^k - 2u_j^k + u_{j-1}^k), \qquad u_0^k = u_\ell, \quad u_N^k = u_r.$$

You can implement this directly with a for loop:

```
# code sketch:
c = beta*dt/h**2
n = len(x) - 1 # x = (x_0, ... x_n)
u = f(x[1:n])  # u at interior points
while t < t_final:
    for j in range(1, n-2):
        unext[j] = u[j] + c*(u[j+1]-2*u[j]+u[j-1])
    # eqs. with boundary terms
    unext[0] = u[0] + c*(u[1] - 2*u[0] + ul)
    unext[n-2] = u[n-2] + c*(ur - 2*u[n-2] + u[n-3])
    u[:] = unext[:]
    t += dt
```





- u: u at current t
- unext: space for u at next t
- n: grid points $x_0, \cdots, x_n$
- x_points: The array of x_j's

Euler's method (directly)

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^k - 2u_j^k + u_{j-1}^k), \qquad u_0^k = u_\ell, \quad u_N^k = u_r.$$

This can be simplified by keeping the boundary points in; we compute

$$u = (u_0, \cdots, u_N)$$

but update only $u_1, \cdots, u_{N-1}$. The formula then holds for all (relevant) j.

```
# code sketch:
c = beta*dt/h**2
n = len(x) - 1 # x = (x_0, ... x_n)
u = f(x)  # u at *all* points
while t < t_final:
    for j in range(1, n+1):
        unext[j] = u[j] + c*(u[j+1]-2*u[j]+u[j-1])
    u[:] = unext[:]
    t += dt
```

- Technique can be extended...
- Use fictional 'ghost points' to make the formula always work ($u_{-1}, \cdots$)
- Simplifies loops (no special cases)

Implicit methods...

A problem: there is a **stability constraint**

$$\Delta t < C \Delta x^2$$

or else numerical solutions grow exponentially!
The fix: use a (good) **implicit** method.

Forward Euler (bad stability):

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^k - 2u_j^k + u_{j-1}^k)$$

matrix form: $\mathbf{u}^{(k+1)} = (I + \Delta t D)\mathbf{u}^{(k)} + \mathbf{b}$

Backward Euler (always stable!):

$$u_j^{k+1} = u_j^k + \frac{\beta \Delta t}{h^2}(u_{j+1}^{k+1} - 2u_j^{k+1} + u_{j-1}^{k+1})$$

matrix form: $(I - \Delta t D)\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \mathbf{b}$

Implicit - at each step, we must solve a **tridiagonal** linear system!