Notas de aula

# Introdução à Física Computacional

Prof. Gerson – UFU – 2019

Atendimento:

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- Horário: sextas-feiras 16:00 – 16:50

# Boundary value problems

wave-equation

$$\frac{\partial^2}{\partial t^2} y(x,t) = c^2 \frac{\partial^2}{\partial x^2} y(x,t)$$

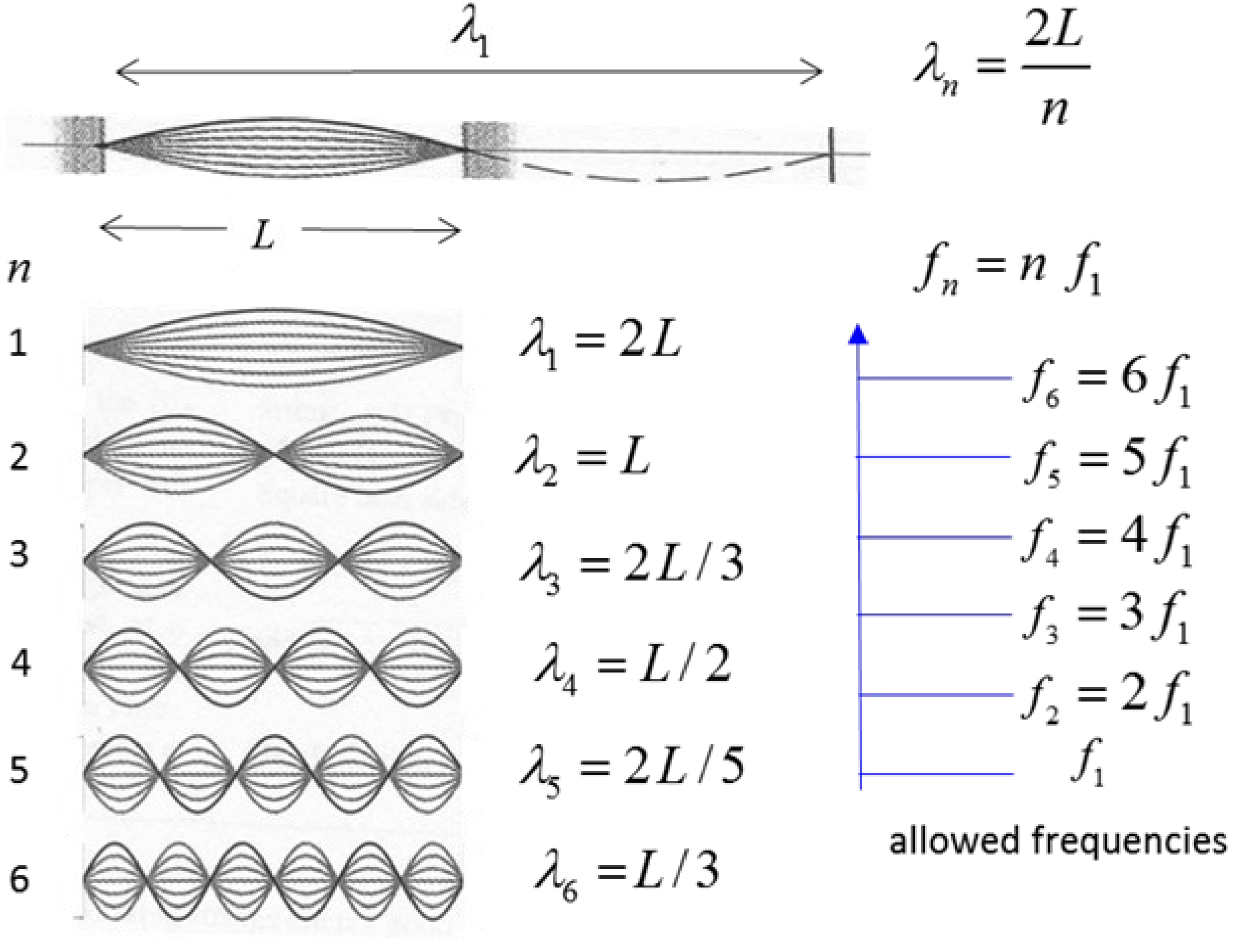
Fourier t → w

$$-\omega^2 y(x,\omega) = c^2 \frac{\partial^2}{\partial x^2} y(x,\omega)$$

as an eigenvalue problem

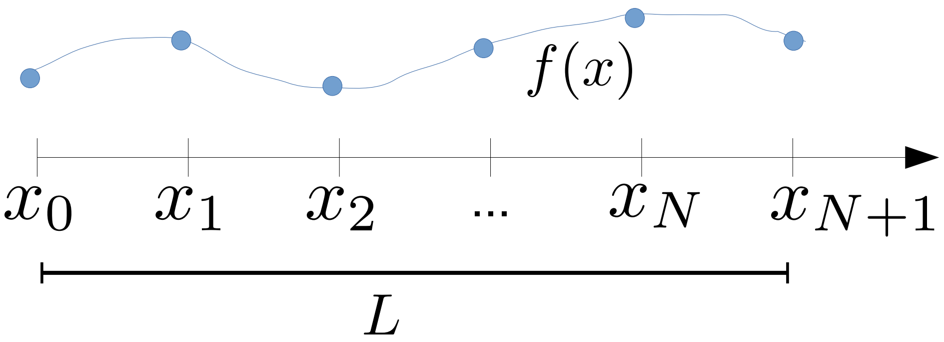
$$-\frac{\partial^2}{\partial x^2} y(x,\omega) = \alpha y(x,w)$$

$$\alpha = \frac{\omega^2}{c^2}$$



# Finite differences

Consider a function f(x) on a discrete lattice




The N points are set as $x_j = x_0 + j\Delta x$

and size L $x_{N+1} = x_0 + L$

This give us → $\Delta x = \dfrac{L}{N+1}$

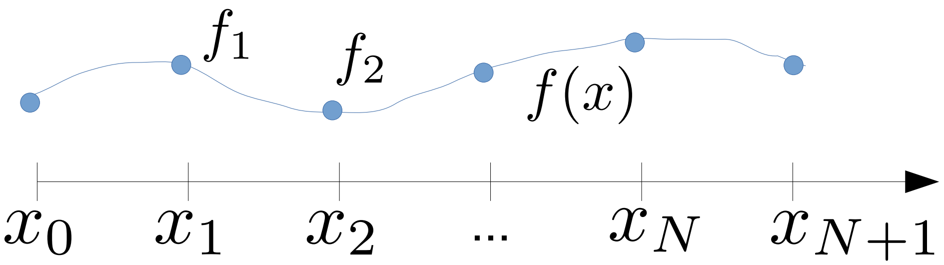
The Taylor expansions of f(x ± Δx) for Δx → 0 are

$$f(x+\Delta x) \approx f(x) + \Delta x\ f'(x) + \frac{\Delta x^2}{2} f''(x) + \frac{\Delta x^3}{3!} f'''(x) + \mathcal{O}(\Delta x^4)$$

$$f(x-\Delta x) \approx f(x) - \Delta x\ f'(x) + \frac{\Delta x^2}{2} f''(x) - \frac{\Delta x^3}{3!} f'''(x) + \mathcal{O}(\Delta x^4)$$

# Finite differences

Matrix representation of d²/dx²




Add the Taylor expansions from the previous page, to obtain

$$f''_n = \frac{f_{n-1} - 2f_n + f_{n+1}}{\Delta x^2}$$

Apply rule for n=1 .. N (inner points)

$$f''_1 = \frac{f_0 - 2f_1 + f_2}{\Delta x^2}$$

$$f''_2 = \frac{f_1 - 2f_2 + f_3}{\Delta x^2}$$

$$f''_3 = \frac{f_2 - 2f_3 + f_4}{\Delta x^2}$$

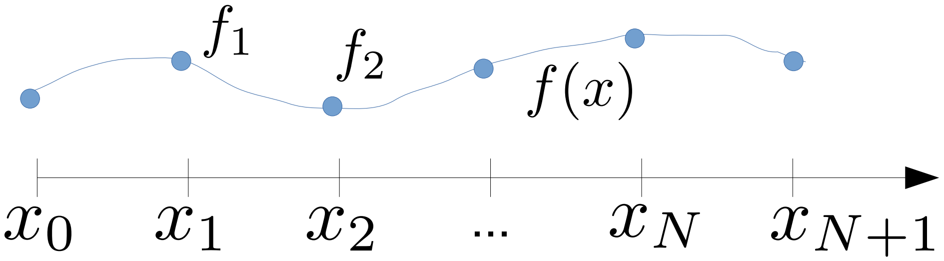
It takes a matrix form

$$\frac{\partial^2}{\partial x^2}\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} + \cancel{\frac{1}{\Delta x^2}\begin{pmatrix} f_0 \\ 0 \\ \vdots \\ f_{N+1} \end{pmatrix}}$$

vanishing boundary conditions: $f_0 = f_{N+1} = 0$

# Finite differences

Matrix representation of d²/dx²

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vanishing boundary conditions: $f_0 = f_{N+1} = 0$

# Homework

Find the matrix representations of the 1st derivative $\dfrac{df(x)}{dx}$ considering:

a) the forward form of the finite differences
b) the backwards form
c) the symmetric form

In all cases, consider also the boundary conditions:

i) vanishing boundary condition (like in the previous slide)
ii) periodic boundary conditions: $x_{N+1} = x_1$, and $x_0 = x_N$

Also… apply the periodic boundary conditions to the 2nd derivative

# The wave-equation in 1D

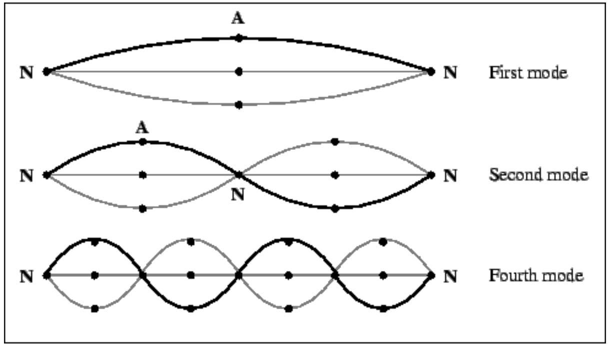
Already considering the Fourier transform t → w

$$-\frac{\partial^2}{\partial x^2} y(x,\omega) = \alpha y(x,w) \qquad \alpha = \frac{\omega^2}{c^2}$$

Representing y(x,w) → y ($x_n$, w) on a discrete lattice

$$-\frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix} = \alpha \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix}$$

# The wave-equation in 1D

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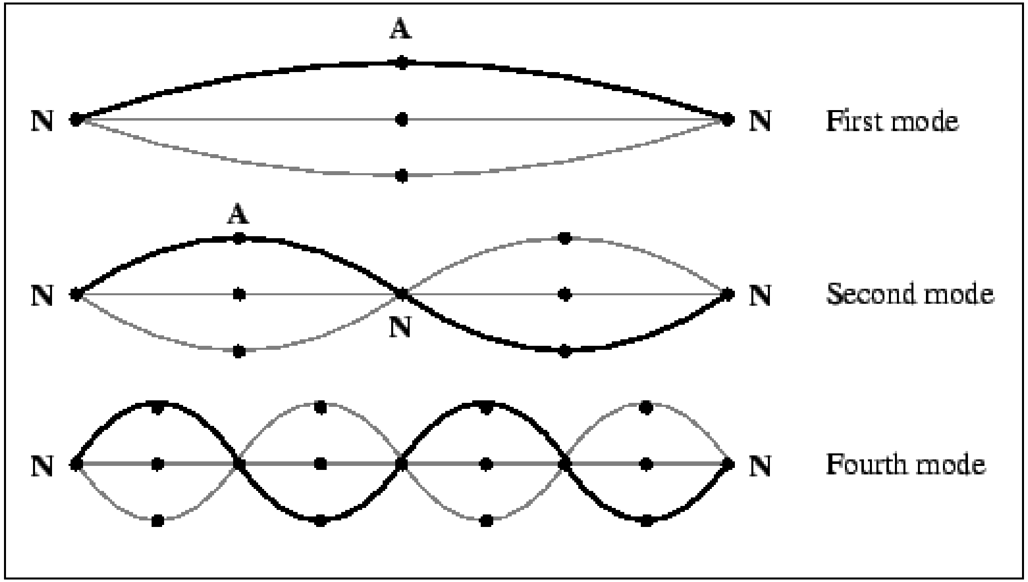
$$-\frac{\partial^2}{\partial x^2} y(x,\omega) = \alpha y(x,w) \qquad \alpha = \frac{\omega^2}{c^2}$$

Representing y(x,w) → y ($x_n$, w) on a discrete lattice … simplifying it

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix} = [\alpha \Delta x^2] \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix}$$

Use numpy.linalg to find the eigenvalues and eigenvectors

# Plot the eigenvectors




Notice that the extreme points are missing: $x_0$ and $x_{N+1}$ → boundary conditions

Tip! Use the numpy functions to build the matrix:

→ np.eye(…) → np.ones(…) → np.diag(…, k = {-1,0,1})

# Wave-equation in 1D: time-evolution

What's is behind the Fourier transform?

$$\frac{\partial^2}{\partial t^2} y(x,t) = c^2 \frac{\partial^2}{\partial x^2} y(x,t) \longrightarrow -\frac{\partial^2}{\partial x^2} y(x,\omega) = \alpha y(x,w)$$

Assume $\varphi_n(x)$ are the eigenvectors of $-d^2/dx^2$ with eigenvalues $\alpha_n = (w_n/c)^2$

Ansatz: $y(x,t) = \sum_n a_n e^{-i\omega_n t} \varphi_n(x)$ $\leftarrow$ satisfies the wave-equation

At t = 0 the wave has an initial form $\rightarrow$ $y(x,0) = y_0(x)$ (initial condition)

Fourier's trick gives $a_n = \int \varphi_n^\dagger(x) y_0(x) dx$

animate!?

# Schrödinger equation

The time-independent equation is identical to the wave equation after the Fourier transform
But let's add a potential V(x)

Use: $\hbar = 1$
$m = 1$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x) + V(x)\varphi(x) = E\varphi(x)$$

The 2nd derivative has the same matrix representation as before, and V(x) is simply

$$V(x)\varphi(x) \rightarrow \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & V_{N-1} & 0 \\ 0 & 0 & 0 & 0 & V_N \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-1} \\ \varphi_N \end{pmatrix}$$

Try it for:

$$V(x) = 0$$

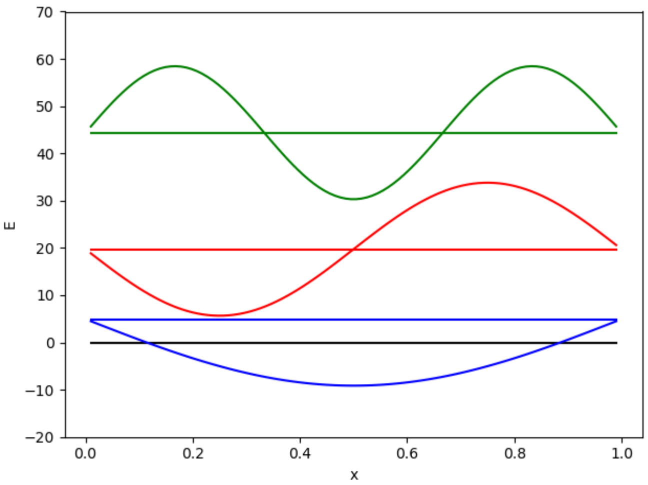
$$V(x) = \frac{1}{2}kx^2$$

$$V(x) = -V_0 \sin(\frac{3\pi x}{L})$$

Use vanishing boundary conditions

# Schrödinger equation → solutions

$$V(x) = 0$$

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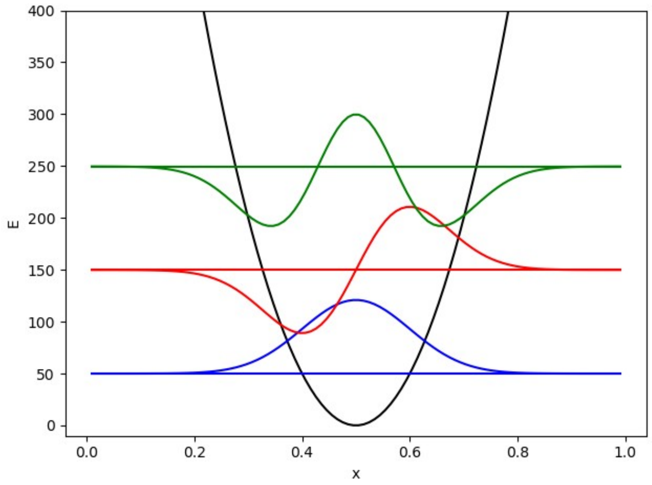


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