Ordinary Differential Equations

- Types of Ordinary differential equations.
- Euler's method.

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- Examples :

$$
\begin{aligned}
m\frac{d^2x(t)}{dt^2} &= -\,kx(t) \\
i\hbar\frac{\partial\psi(x,t)}{\partial t} &= -\,\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)
\end{aligned}
$$

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- Initial value problem vs boundary value problem vs eigenvalue problem.

Simple Harmonic Oscillator

$$m\frac{d^2x(t)}{dt^2} = -kx(t)$$
$$x(t=0) = x_0$$
$$\left.\frac{dx}{dt}\right|_{t=0} = v_0$$

is initial value problem for the second order ordinary linear homogeneous differential equation

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- The ordinary differential equations (ODE) – have functions of one only independent variable.
  Example: stationary Schrödinger equation
- The partial differential equations (PDE) – have functions of several independent variables.
  Example: time dependent Schrödinger equation for $\psi(\mathbf{r}, t)$

- A linear differential equation – all of the derivatives appear in linear form and none of the coefficient depends on the dependent variable

$$a_0 x(t) + a_1 \frac{dx}{dt} + a_2 \frac{d^2x}{dt^2} + \ldots = c$$

Example:

$$m \frac{d^2x(t)}{dt^2} = -kx(t)$$

Non-linear differential equation

- A nonlinear differential equation – if the coefficients depend on the dependent variable, OR the derivatives appear in a nonlinear form:
  Examples:

$$\frac{dx}{dt}\frac{d^2x}{dt^2} - x(t) = 0$$
$$t^2\frac{d^2x}{dt^2} - x^2(t) = 0$$

Order of the ODE

- The order n of an ordinary differential equation is the order of the highest derivative appearing in the differential equation

$$t^2 \frac{d^2x(t)}{dt^2} - x(t) = 0 \quad \text{second order}$$
$$t \frac{d^3x(t)}{dt^3} - \frac{dx(t)}{dt} = 0 \quad \text{third order}$$

General or partial solution

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- Partial solutions:

$$x(t) = 2.0e^t$$
$$x(t) = 4.8e^t$$

- A homogeneous equation: the each term contains either the function or its derivative, but no other functions of independent variables:

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- A homogeneous equation: the each term contains either the function or its derivative, but no other functions of independent variables:

$$m\frac{d^2x(t)}{dt^2} - kx(t) = 0$$

- A non-homogeneous equation: contains additional term (source terms, forcing functions) which do not involve the dependent variable:

$$m\frac{d^2x(t)}{dt^2} - kx(t) = F_0\cos(\omega t)$$

Three major categories of ODE

- Initial-value problems – involve time-dependent equations with given initial conditions:

$$m\frac{d^2x(t)}{dt^2} - kx(t) = 0 \qquad x(t=0) = x_0, \quad \left.\frac{dx}{dt}\right|_{t=0} = v_0$$

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- Boundary-value problems – involve differential equations with specified boundary conditions:

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In reality, a problem may have more than just one of the categories active.

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- Propagation problems – are initial value problems in open domains where the initial values are marched forward in time (or space) . The order may be one or greater. The number of initial values must be equal to the order of the differential equation.

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- Eigenproblems – are a special type of problems where the solution exists only for special values of a parameter.

Converting n^{th} order to n linear equations

Any n^{th} order linear differential equation can be reduced to n coupled first order differential equations. Example:

$$m\frac{d^2x(t)}{dt^2} - kx(t) = 0$$

is the same as:

$$\begin{aligned} \frac{dx(t)}{dt} &= v(t) \\ m\frac{dv(t)}{dt} &= -kx(t) \end{aligned}$$

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- Solving the resulting algebraic FDE

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Three groups of FDs for solving initial-value ODEs

- Single point methods advance the solution from one grid point to the next grid point using only the data at a single grid point. (most significant method – 4th order Runge-Kutta).
- Extrapolation methods evaluate the solution at a grid point for several values of grid size and extrapolate those results to get for a more accurate solution.
- Multipoint methods advance the solution form one grid point to the next using the data at several known points (4th order Adams-Bashforth-Moulton method).

Using the Taylor series for x_{n+1} using the grid point n.

truncation error $\mathcal{O}(\Delta t^{m+1})$

Using the Taylor series for x_{n+1} using the grid point n.

$$x_{n+1} = x_n + x'|_n \Delta t + \frac{1}{2} x''_n (\Delta t)^2 + \ldots + \frac{1}{m!} x^m|_n \Delta t^m + R^{m+1}$$

$$R^{m+1} = \frac{1}{(m+1)!} x^{m+1}(\tau) \Delta t^{m+1} \quad t \leq \tau \leq t + \Delta t$$

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Solving for $x'|_n$ yields:

$$x'|_n = \frac{x_{n+1} - x_n}{\Delta t} - \frac{1}{2} x''|_n \Delta t - \frac{1}{6} x'''|_n (\Delta t)^3$$

Finite difference approximations

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- a first - order finite difference approximation:

$$x'|_n = \frac{x_{n+1} - x_n}{\Delta t} \quad \mathcal{O}(\Delta t)$$

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- A second-order centered difference approximation of x' at point $n + \frac{1}{2}$:

$$x'|_{n+\frac{1}{2}} = \frac{x_{n+1} - x_n}{\Delta t} \quad \mathcal{O}(\Delta t^2)$$

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Substitute into the ODE and solve for x_{n+1}:

$$x_{n+1} = x_n + f(x_n, t_n)\Delta t \qquad \text{Explicit finite difference}$$
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The explicit Euler method for ODE

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Explicit finite difference (first order):

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then

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- The global error accumulated after n steps $\mathcal{O}(\Delta t)$
- Problem: the method is conditionally stable for $\Delta t \leq \Delta t_{cr}$.

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- Implicit (since $f(x_{n+1}, t_{n+1})$ does depend on x_{n+1})
- The implicit Euler is unconditionally stable.
- However, if $f(x, t)$ is non-linear, then we need to use one of the methods for solving non-linear equations.

Stability of Euler method

Consider the 'linear test equation':

$$\frac{dx(t)}{dt} = \lambda x(t)$$

where $\lambda \in \mathbb{C}$ and $x(t=0) = x_0 \neq 0$.
The exact solution of this equation is:

$$x(t) = x_0 e^{\lambda t}$$

For $\Re(\lambda) < 0$, then the solution $x(t \to \infty) \to 0$.

Stability of explicit Euler equation

$$x_{n+1} = x_n + \lambda \, \delta t \, x_n$$
$$x_{n+1} = (1 + \lambda \, \delta t)^n x_0$$

So for the case when $\Re(\lambda) < 0$:

$$|1 + \lambda \, \delta t| < 1$$

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If we restrict that $\lambda \in \mathbb{R}$:

$$\begin{aligned} -1 < 1 + \lambda\,\delta t &< 1 \\ -2 < \lambda\,\delta t &< 0 \\ 0 < \delta t &< -\frac{2}{\lambda} \end{aligned}$$

(as $\delta t > 0$ and $\lambda < 0$).

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(as $\delta t > 0$ and $\lambda < 0$).
The condition of stability is:

$$\delta t < -\frac{2}{\lambda}$$

Stability of implicit Euler equation

$$x_{n+1} = x_n + \lambda\,\delta t\,x_{n+1}$$
$$x_{n+1} = \frac{1}{1-\lambda\,\delta t}x_n$$
$$x_{n+1} = \left(\frac{1}{1-\lambda\,\delta t}\right)^n x_0$$

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So for the case when $\Re(\lambda) < 0$:

$$\left|\frac{1}{1-\lambda\,\delta t}\right| < 1$$

If we restrict $\lambda \in \mathbb{R}$, the negativity of λ implies that the single-step amplification factor $1/(1+|\lambda|\delta t)$ is $<$ 1, irrespective of δt. Thus, implicit Euler method is unconditionally stable.