

Ordinary Differential Equations – IVP I

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IL PRESENTE MATERIALE È RISERVATO AL PERSONALE DELL'UNIVERSITÀ DI BOLOGNA E NON PUÒ ESSERE UTILIZZATO AI TERMINI DI LEGGE DA ALTRE PERSONE O PER FINI NON ISTITUZIONALI

Numerical Methods for ODE

- One-step Methods
 - Euler's Method
 - Analysis of the one-step methods
 - Runge-Kutta Methods
- Multi-step Methods
 - Adams-Bashforth
 - Adams-Moulton
 - Predictor-Corrector
- Systems of ODE
- Stability
- Stiff Problems



Leonhard Euler (1707-1783),

Martin Kutta Carl David Runge (1856-1927)





J.C. Adams (1819-1882)



"...It is by looking into the same problem from different points of view that one arrives to a complete insight of it."

Euler

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Ordinary Differential Equations ODE

Scalar Linear ODE of the first order

$$y'(x) + p(x)y(x) = f(x)$$

The term **order** indicates the maximum order of differentiation of the unknown function that is present in the equation. The ODE is said to be **homogeneous** if f(x) = 0:

$$y'(x) + p(x)y(x) = 0$$

Theorem: Solution of the homogeneous equation The set of solutions is given by the family of functions in the form: $y(x) = Ce^{-\int p(x)dx}$

Ordinary Differential Equations ODE

Procedure to solve a homogeneous ODE with separable variables:

$$y'(x) + p(x)y(x) = 0$$

$$\frac{dy}{dx} = -p(x)y(x) \qquad \implies \qquad \frac{1}{y(x)}dy = -p(x)dx$$
$$\int \frac{1}{y(x)}dy = -\int p(x)dx \qquad \implies \qquad \log(y(x)) = -\int p(x)dx + c$$

The general integral is: $y(x) = e^{-\int p(x)dx + c} = Ce^{-\int p(x)dx}$

where *C* is a *constant* of *integration*

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Constant coefficient linear ODE

In general, a linear ODE with constant coefficients (λ)

 $\begin{cases} y'(x) = \lambda y(x) \\ y(x_0) = x_0 \end{cases}$ has solution: $y(x) = y_0 e^{\lambda (x - x_0)}$



$$y'(t) = -5y(t)$$

solution:
$$y(t) = ce^{-5t}, c \text{ constant}$$

$$y(0) = 1 \rightarrow y(t) = e^{-5t}$$

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Ordinary Differential Equations ODE

A first order diff. equation takes the general form

$$y'(x) = f(x, y(x)) \quad \forall x \in I \equiv [a, b]$$

f(x,y(x)) is a *linear* or *nonlinear* function on y. The differential equation is satisfied by a family of functions. The **initial condition**

$$y(x_0) = y_0, \quad x_0 \in [a, b]$$

isolates one of these solutions (solution of the Initial Value Problem IVP)



Initial Value Problems (IVP)

CAUCHY PROBLEM (or IVP)

Determine the solution of an ordinary differential, scalar or vector equation, completed by appropriate initial conditions.

IVP associated with an ODE of the first order

Determine a function y(x), continuous and differentiable on the interval I in R such that

$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \equiv [a, b] \\ y(x_0) = y_0 & x_0 \in [a, b] \end{cases}$$



A first order SYSTEM OF m ORDINARY EQUATIONS:

$$\begin{cases} y'_{1}(x) = f_{1}(x, y_{1}(x), ..., y_{m}(x)) \\ y'_{2}(x) = f_{2}(x, y_{1}(x), ..., y_{m}(x)) \\ \\ y'_{m}(x) = f_{m}(x, y_{1}(x), ..., y_{m}(x)) \end{cases} \begin{cases} y_{1}(x_{0}) = y_{1,0} \\ y_{2}(x_{0}) = y_{2,0} \\ \\ y_{m}(x_{0}) = y_{m,0} \end{cases}$$

Each unknown function y_i satisfies an ODE with initial condition. All initial conditions are specified at the same value of the independent variable x. In compact form:

$$\begin{cases} Y'(x) = F(x, Y(x)) \\ Y(0) = Y_0 \end{cases}$$

 $Y'(x) = (y'_{1}(x), \dots, y'_{m}(x)) \quad Y_{0}(x) = (y_{1,0}(x), \dots, y_{m,0}(x))$

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Constant coefficient linear system of ODEs

Linear first order system of ODEs

$$y'(x) = A(x)y(x) + f(x) \qquad A(x) \in \mathbb{R}^{mxm}, \ f \in \mathbb{R}^m$$

- A linear system of ODEs with constant coefficients y'(x) = Ay(x) + f(x) $A \in \mathbb{R}^{mxm}$, $f \in \mathbb{R}^{m}$ has solution $y(x) = y_0 e^{A(x-x_0)} + \int_{x_0}^x e^{A(x-\tau)} f(\tau) d\tau$
- The system of ODEs is **homogeneous** if f(x) = 0
- Assume A has constant coefficients and f(x) = 0,

$$y'(x) = Ay(x)$$

$$y(x) = y_0 e^{A(x-x_0)}$$

then the solution is



Constant coefficient linear system of ODEs

Procedure to solve a homogeneous system of ODEs:

$$\begin{cases} y'(x) = Ay(x) & \forall x \in I \equiv [a,b] \\ y(x_0) = y_0 & x_0 \in [a,b] \end{cases}$$

When A is diagonalizable, compute the eigenvalues and the eigenvectors of the coefficient matrix A such that



Constant coefficient linear system of ODEs

This is a decoupled set of m scalar equations

$$\begin{cases} d'_{l}(x) = \lambda_{l} d_{l}(x) \\ d_{l}(x_{0}) = \eta_{l} \end{cases} \quad l = 1, 2, ..., m \quad \text{with exact solution} \\ d_{l}(x) = \eta_{l} e^{\lambda_{l}(x - x_{0})} \end{cases}$$

The solution of the original (coupled) ODE system is

$$y(x) = Hd(x) = \sum_{l=1}^{m} \eta_{l} e^{\lambda_{l} (x-x_{0})} \xi_{l} = He^{\Lambda(x-x_{0})} H^{-1} y_{0}$$
$$= y_{0} e^{A(x-x_{0})}$$



nth-order Differential Equation

Any *m*th-order differential equation, requires *m* conditions to obtain a unique solution

$$y^{(m)}(x) = f(x, y(x), y'(x), ..., y^{(m-1)}(x))$$
$$y(x_0) = y_{1,0}$$
$$y'(x_0) = y_{2,0}$$

$$y^{(m-1)}(x_0) = y_{m,0}$$

and it is equivalent to a **system of m equations** of the first order:

nth-order Differential Equation

Let:

$$\begin{cases}
z_{1}(x) = y(x) \\
z_{2}(x) = y'(x) \\
\dots \\
z_{m}(x) = y^{(m-1)}(x)
\end{cases}$$

$$\begin{cases}
z_{1}(x) = z_{2}(x) \\
\dots \\
z_{m-1}(x) = z_{m}(x) \\
z_{m}(x) = f(x, z_{1}(x), z_{2}(x), \dots, z_{m-1}(x))
\end{cases}$$

$$\begin{cases}
z_{1}(x_{0}) = y_{1,0} \\
z_{2}(x_{0}) = y_{2,0} \\
\dots \\
z_{m}(x_{0}) = y_{m,0}
\end{cases}$$



Linear second order differential equation for a vibrating system with springs:



The initial conditions are $x(0) = x_0$ and x'(0) = 0.



Let's rewrite the equation:

$$\frac{d^2x}{dt^2} = -\left(\frac{c}{m}\frac{dx}{dt} + \frac{k}{m}x\right)$$
$$z_1(t) = x(t)$$

$$z_2(t) = \frac{dx}{dt}$$



The equation can be rewritten as a system of two equations of the first order

$$\frac{dz_1}{dt} = z_2(t)$$
$$\frac{dz_2}{dt} = -\left(\frac{c}{m}z_2(t) + \frac{k}{m}z_1(t)\right)$$

The initial conditions are $z_1(0) = x_0$ and $z_2(0) = 0$.



Second order ODE: Example

Predict the motion of a swinging pendulum of mass m hanging from a wire of length L in the absence of friction.

Non-linear second order ODE in θ (the angle with the vertical):

$$\mathcal{G}'' + \frac{g}{L}\sin\mathcal{G} = 0$$

Convert into a system of two non-linear ODEs of the first order



$$\begin{cases} z_1 = \vartheta \\ z_2 = \vartheta' \end{cases} \begin{cases} \frac{dz_1}{dt} = \vartheta' = z_2 \\ \frac{dz_2}{dt} = -\frac{g}{L} \sin(z_1) \end{cases}$$



Lipschitz Function

Definition Rudolph Sigismund Lipschitz (1832-1903)

A function f :I -> R is Lipschitz (short Lip) in the interval I if it exists a constant L such that, for whatever pair of values (y_1, y_2) in I × I, the following upper bound holds

$$f(y_1) - f(y_2) | \le L |y_1 - y_2|$$

 This is equivalent to saying that the incremental ratio of f in the interval I is limited

$$\frac{\left|f(y_1) - f(y_2)\right|}{\left|y_1 - y_2\right|} \le L$$

 L is the Lipschitz constant for f if it is the lower bound of the constants L for which the inequalities hold.

(f differentiable -> f Lip., f Lip. -> f continuous)



Theorem :

Existence and uniqueness of solutions

Assume that the function f(x,y) is

1. continuous with respect to both its arguments;

2. Lipschitz-continuous with respect to its second argument, that is, there exists a positive constant L (named Lipschitz constant) such that

$$\|f(x,y_1) - f(x,y_2)\| \le L \|y_1 - y_2\|$$
 $x \in I = [a,b], \forall y_1, y_2 \in \mathbb{R}.$

Then the solution y = y(x) of the Cauchy problem exists, is unique and belongs to C¹(I):

$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \\ y(x_0) = y_0 \\ y(x) \in C^1[a, b] \end{cases}$$



- The Lipschitz constant measures how much f(x,y(x)) changes if we perturb y (at some fixed time x)
- Example



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IVP is a well-posed problem

The Cauchy problem, when the function f(x,y) verifies the Lipschitz condition, is a **well posed problem**; that is, the solution has **existence**, **uniqueness** and has a **continuous dependence on the initial data**.

From the numerical point of view, the continuous dependence on data is essential, since one works on approximate quantities, but it may not be sufficient for an adequate numerical approximation.

In fact, the problem must be **well conditioned:** small changes in the data leads to small variations on the results.

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Stability vs. Conditioning

- The terms stability and conditioning are used with a variety of meanings in Numerical Analysis. They have in common the general concept of the response of a set of computations to perturbations arising from
 - the data,
 - the specific arithmetic used on computers.
- In other words, a numerical algorithm is not only perturbed by the *errors in the data*, but also with respect to the *errors arising in the process of computations*.
- They are not synonymous.





- In Mathematics the notion of stability derives from the homonymous notion in mechanics.
- It regards the behavior of the motion of a system when it is moved away from the equilibrium.
- Three ingredients enters in the definition, i.e.
 - the existence of a reference solution, i.e. the equilibrium;
 - the perturbation of the initial status (the initial conditions);
 - the duration of the motion, which is supposed to be infinite.





- Many problems, however, do not last for a long (in principle, infinite) time, and/or do not have an equilibrium.
- The above concept of stability do not apply, as it stands.
- The numerical analysts would like to know if the dependence of the solution on data, although continuous (if the problem is well-posed), may result *disastrous* for the error growth.
- This requires the notion of *Conditioning*.



"The most fundamental is the distinction between instability in the underlying mathematical problem and instability in an algorithm for the (exact or approximate) treatment of the problem".

Dahlquist

Stiffness is the ill-conditioning of the continuous problem



III-Conditioning: Iinear system of ODEs

The study of conditioning can be done exactly with linear ODE systems of the type:

(*)
$$\begin{cases} y'(x) = Ay(x) + g(x) & \forall x \in I \equiv [a,b] \\ y(x_0) = y_0 & x_0 \in [a,b] \end{cases}$$

Let consider the perturbed problem

(**)
$$\begin{cases} z'(x) = Az(x) + g(x) \\ z(x_0) = y_0 + \varepsilon \\ \text{where } z(x) = y(x; x_0 + \varepsilon) \end{cases}$$

Let $\delta(x) = z(x) - y(x)$ subtracting (*)-(**) we have

III-Conditioning:
linear system of ODEs
(***)
$$\begin{cases} \delta'(x) = A \delta(x) \\ \delta(x_0) = \varepsilon \end{cases}$$
If $\delta(x_0) = z(x_0) - y(x_0)$ is small then
 $\delta(x) = z(x) - y(x)$ is small too
 $\delta(\overline{x}) = y(x)$ is small too
 $\delta(\overline{x}) = y(x)$ is small too

Solve (***) by diagonalization $A = H\Lambda H^{-1}$ $H = (\xi_1, \xi_2, ..., \xi_m)$



III-Conditioning: Iinear system of ODEs

with solution

$$\delta(x) = \sum_{l=1}^{m} \eta_l e^{\lambda_l (x-x_0)} \xi_l$$

The eigenvalues of the matrix A characterize the response of the system to the introduction of initial value perturbations.

$$\|\delta(x)\| \to \infty$$
 for $x \to \infty$ when $\operatorname{Re}(\lambda_l) > 0$ at least for one index 1
 $\|\delta(x)\| \to 0$ for $x \to \infty$ when $\operatorname{Re}(\lambda_l) < 0$ for $l = 1, 2, ..., m$

When all the eigenvalues of the matrix A have negative real parts we define the problem Asymptotically Stable Problem (AS)

The y(x) curve is simply called stable if $\|\delta(x)\|$ it is kept limited



Example

Given the IVP system

$$\begin{cases} y_1'(x) = y_2 \\ y_2'(x) = y_1 \end{cases} \begin{cases} y_1(0) = 1 \\ y_2(0) = -1 \end{cases}$$

Eigenvalues and eigenvectors:

$$\lambda_1 = 1, \lambda_2 = -1 \qquad H$$



• General solutions:

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} c_1 e^x + \begin{bmatrix} 1 \\ -1 \end{bmatrix} c_2 e^{-x}$$

 ρ^{-x}

• Replace initial conditions:

$$y_1(x) = e^{-x}, \qquad y_2(x) = -$$



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• perturbing the initial conditions:

$$\tilde{y}_1(0) = 1 + \varepsilon, \qquad \tilde{y}_2(0) = -1$$

$$\begin{cases} a_1 + a_2 = 1 + \varepsilon \\ a_1 - a_2 = -1 \end{cases} \qquad a_1 = \frac{\varepsilon}{2}, \qquad a_2 = 1 + \frac{\varepsilon}{2} \end{cases}$$

• Solution of the perturbed problem

$$\widetilde{y}_1 = \frac{\varepsilon}{2}e^x + \left(1 + \frac{\varepsilon}{2}\right)e^{-x}, \qquad \widetilde{y}_2 = \frac{\varepsilon}{2}e^x - \left(1 + \frac{\varepsilon}{2}\right)e^{-x}$$

The initial error is multiplied by the amplification factor e^x so the problem is unstable.





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III-Conditioning: nonlinear system of ODEs $(x) = f(x, y(x)) \quad \forall x \in I \equiv [a, b]$

$$\begin{cases} y'(x) = f(x, y(x)) & \forall x \in I \equiv [a, b] \\ y(x_0) = y_0 & x_0 \in [a, b] \end{cases}$$

Perturbed problem

$$\begin{cases} z'(x) = f(x, z(x)) \\ z(x_0) = y_0 + \varepsilon \end{cases} \quad \text{set} \quad z(x) = y(x) + \delta(x) \end{cases}$$

Consider the Taylor expansion of the perturbed function

at (x,y(x))

$$f(x,z(x)) = f(x,y(x) + \delta(x))$$

$$f(x,z(x)) = f(x,y(x)) + f_y(x,y(x))\delta(x) + O(||\delta||^2)$$
assume $O(||\delta||^2)$ negligible



III-Conditioning: nonlinear system of ODEs

Consider only the linear part

$$\begin{cases} y'(x) + \delta'(x) \cong f(x, y(x)) + f_y(x, y(x)) \delta(x) \\ y(x_0) + \delta(x_0) = y_0 + \varepsilon \end{cases}$$

we get

$$\begin{cases} \delta'(x) \cong f_y(x, y(x)) \delta(x) \\ \delta(x_0) = \varepsilon \end{cases}$$

REMARK: Jacobian matrix of f wrt y has elements

$$\left\{f_{y}(x, y(x))\right\}_{ii} = \left\{J_{f}\right\}_{ij} = \frac{\partial f_{i}(x, y)}{\partial y_{i}}$$



III-Conditioning: nonlinear system of ODEs

Assuming that $f_y(x,y(x))$ is almost constant, i.e.

$$f_{y}(x,y(x)) \cong f_{y}(x_{0},y_{0})$$

we can say that, as a first approximation, propagation of the initial error ϵ is defined by

$$\begin{cases} \delta'(x) \cong f_y(x_0, y_0) \delta(x) \\ \delta(x_0) = \varepsilon \end{cases}$$
$$\delta(x) = \varepsilon e^{f_y(x - x_0)}$$



Ill-Conditioning: <u>nonlinear system of ODEs</u> $\delta(x) = \varepsilon e^{f_y(x-x_0)}$

 $\|\delta(x)\| \to \infty$ for $x \to \infty$ when $\operatorname{Re}(\lambda_l) > 0$ at least one index 1 $\|\delta(x)\| \to 0$ for $x \to \infty$ when $\operatorname{Re}(\lambda_l) < 0$ for l = 1, 2, ..., m

• Scalar nonlinear IVP:

- If $f_y < 0$ then the IVP is well-conditioned otherwise is ill-conditioned
- System of nonlinear IVPs

if all the eigenvalues λ_{l} of the Jacobian matrix f_{y} have a negative real part then the IVP system is ill-conditioned well-conditioned otherwise



III-Conditioning: nonlinear system of ODEs

The study of the propagation of an initial perturbation it was possible assuming:

- the term $O(\|\delta\|^2)$ is negligible
- the Jacobian is constant

In reality these hypotheses are often not verified and the behavior of $\delta(x)$ may not be well represented by the eigenvalues of $f_y(x_0, y_0)$.



NUMERICAL METHODS for ODE: discretization

Determine an approximate solution of the Cauchy Problem:

$$\begin{cases} y'(x) = f(x, y(x)) & x \in I \\ y(x_0) = y_0 \end{cases}$$

Basic Idea

- Subdivide the integration interval I into N_h intervals of length h = I/N_h; h is called the discretization step.
- Consider the sequence of points x_j=x₀+jh with j = 0,1,2, ... named nodes.
- Approximate the values of the solution y(x_j) at the nodes x_j and call this approximation u_j. j=0,1,2,....

The sequence of points (x_j,u_j) is the numerical solution that approximates the solution y(x) in I



NUMERICAL METHODS for ODE: discretization

$$\begin{cases} y'(x) = f(x, y(x)) & x \in I \\ y(x_0) = y_0 \end{cases}$$

Fundamental theorem of integral calculus

$$y(x'') - y(x') = \int_{x'}^{x} f(x, y(x)) dx \quad x_0 \le x' < x''$$

Let x' and x" be two nodes of the discretization:

$$x' = x_i$$
 $x'' = x_i + h$

Then the right term is numerically integrated with a quadrature formula.



Some numerical Methods for ODE

$$\begin{split} u_{j+1} - u_{j} &= h \ f(x_{j}, u_{j}) & \text{Forward Euler} \\ u_{j+1} - u_{j} &= h \ f(x_{j+1}, u_{j+1}) & \text{Backward Euler} \\ u_{j+1} - u_{j-1} &= 2h \ f(x_{j}, u_{j}) & \text{Midpoint method} \\ (also called the leapfrog method) \\ u_{j+1} - u_{j} &= \frac{h}{2} [f(x_{j}, u_{j}) + f(x_{j+1}, u_{j+1})] & \text{Trapezoidal} \\ (Crank-Nicolson) \\ u_{j+1} - u_{j-1} &= \frac{h}{3} [f(x_{j-1}, u_{j-1}) + 4f(x_{j}, u_{j}) + f(x_{j+1}, u_{j+1})] \\ \end{split}$$

Simpson



General concepts for numerical ODE methods

- 1. number of steps
- 2. Explicit or implicit approaches
- 3. stability property
- 4. convergence property
- 5. order of **convegence**



General concepts for numerical ODE methods

1. The number of steps

A numerical method is **one-step** if $\forall j \ge 0$ (**One step** u_{j+1} depends only on u_{j} .

A numerical method is **p-step** if $\forall j \ge p-1$ u_{j+1} depends on: $(p \ge 2)$ Multistep

$$\boldsymbol{\mathcal{U}}_{j}, \boldsymbol{\mathcal{U}}_{j-1}, \dots, \boldsymbol{\mathcal{U}}_{j+1-p}$$

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General concepts for numerical ODE methods

2. Explicit vs Implicit approaches

A method is said to be **explicit** if u_{j+1} is derived directly as a function of the known values u_j , u_{j-1}

$u_{j+1} - u_j = h f(x_j, u_j)$	Forward Euler's Method
$u_{j+1} - u_{j-1} = 2h f(x_j, u_j)$	Midpoint Method

A method is said to be **implicit** if the computation of u_{j+1} depends implicitly on u_{j+1} itself!

$$u_{j+1} - u_j = h f(x_{j+1}, u_{j+1})$$
 Backward Euler's Method

Consequently the implicit methods require at every step solving in general a nonlinear equation for u_{i+1} .

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General concepts for numerical ODE methods

3. Stability Property

A numerical method is said to be **stable** if small variations in the initial values correspond to small variations in the solutions.

Unstable - that is, it amplifies errors

If the numerical method were not stable, the rounding errors introduced on y_0 and propagated in the calculation of $f(x_n, u_n)$ at each step, would make the calculated solution completely meaningless.



General concepts for numerical ODE methods

4. Convergence Property

A numerical method is said to be convergent with respect to h if $\exists C > 0$ independent on h s.t.

$$\left\| y(x_j) - u_j \right\| \le C(h) \quad \forall j \ge 1$$

where C(h) is infinitesimal with respect to h when h tends to zero.

A zero-stable method turns out to be convergent if and only if it is also consistent:

CONVERGENCE = ZERO-STABILITY+CONSISTENCE



General concepts for numerical ODE methods

5. The order of convergence

The accuracy of a convergent method is measured by the infinitesimal order of the error with respect to h.

Specifically, a numerical method converges with order p if

 $\exists C > 0$ independent on h s.t.

$$\|y(x_j)-u_j\| \leq C(h^p) \quad \forall j \geq 1.$$





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