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Initial value problems

$$y'(x) = f(x, y(x)), \qquad (x_0 < x < x_0 + A)$$
$$y(x_0) = y_0 \qquad (\textit{initial condition})$$

(where f is a given bivariate functions which satisfies the Lipschitz condition).

Example (dilution of a solution). Consider a container with volume V filled by e.g. salty water. Start filling clean water in the container at the top continuously, and let the salty water flow out from the container at the bottom. Then obviously the salt solution becomes more and more diluted. The process of dilution is described by the following differential equation:

$$c'(t) = -\frac{Q}{V}c(t)$$

where $c(t)$ is the concentartation of the slt at the time t in the container, Q is the discharge of wate, (inflow water volume per time unit).
Initial condition:

$$c(0) = c_0$$

where c_0 is the initial salt concentration at the time $t = 0$.

Boundary value problems

$$y''(x) = f(x, y(x), y'(x)), \qquad (x_0 < x < x_1)$$
$$y(x_0) = y_0, \quad y(x_1) = y_1 \qquad (\textit{boundary conditions})$$

(where f is a given, trivariate function which satisfies the Lispchitz condition).
As a boundary condition, the derivatives of f or a linear combination of the values and the derivatives can also be prescribed.

Example (electrical current in conductors). Consider a thin, long but not necessarily homogeneous piece of conductor. Connect a voltage source to the endpoints of the conductor. The distribution of the electrical potential along the conductor is described by the following differential equation:

$$(\sigma \cdot U')' = 0 \, ,$$

where $U(x)$ denotes the electrical potential at the point x of the conductor, $\sigma(x)$ is the electrical conductivity here.
The boundary conditions are for instance:

$$U(x_0) = U_0, \quad U(x_1) = U_1$$

where U_0, U_1 are the electrical potentials at the endpoints of the conductor.

Solution principles for initial value problems

Useful tools:

Taylor formula for univariate functions:

$$f(x+h) = f(x) + \frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \ldots = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)}{k!}h^k$$

Taylor formula for bivariate functions:

$$\begin{aligned} f(x+h, y+\delta) = f(x,y) &+ \frac{1}{1!}\left(\frac{\partial f(x,y)}{\partial x}h + \frac{\partial f(x,y)}{\partial y}\delta \right) + \frac{1}{2!}\left(\frac{\partial^2 f(x,y)}{\partial x^2}h^2 + 2\frac{\partial^2 f(x,y)}{\partial x \partial y}h\delta + \frac{\partial^2 f(x,y)}{\partial y^2}\delta^2 \right) + \\ &+ \frac{1}{3!}\left(\frac{\partial^3 f(x,y)}{\partial x^3}h^3 + 3\frac{\partial^3 f(x,y)}{\partial x^2 \partial y}h^2\delta + 3\frac{\partial^3 f(x,y)}{\partial x \partial y^2}h\delta^2 + \frac{\partial^3 f(x,y)}{\partial y^3}\delta^3 \right) + \ldots \\ &+ \frac{1}{k!}\left(\binom{k}{0}\frac{\partial^k f(x,y)}{\partial x^k}h^k + \binom{k}{1}\frac{\partial^k f(x,y)}{\partial x^{k-1}\partial y}h^{k-1}\delta + \ldots + \binom{k}{k}\frac{\partial^k f(x,y)}{\partial y^k}\delta^k \right) = \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{j=0}^{k} \binom{k}{j} \frac{\partial^k f(x,y)}{\partial x^{k-j}\partial y^j} h^{k-j}\delta^j \end{aligned}$$

Computational grid: $x_k := x_0 + kh \quad (k = 0,1,\ldots,N)$, where h is the **stepsize**.
Goal: to approximate the values of the solution y at the gridpoints only.

1. Approximation of the derivatives by finite differences
First-order derivative:

- Forward scheme: $\boxed{y'(x_k) \sim \dfrac{y_{k+1} - y_k}{h}}$ Error: $O(h)$,

  since from Taylor's formula: $y_{k+1} = y(x_{k+1}) = y(x_k + h) = y_k + y'(x_k)h + O(h^2)$

- Backward scheme: $\boxed{y'(x_k) \sim \dfrac{y_k - y_{k-1}}{h}}$ Error: $O(h)$,

  since from Taylor's formula: $y_{k-1} = y(x_{k-1}) = y(x_k - h) = y_k - y'(x_k)h + O(h^2)$

- Central scheme: $\boxed{y'(x_k) \sim \dfrac{y_{k+1} - y_{k-1}}{2h}}$ Error: $O(h^2)$,

  since: $y_{k+1} = y(x_{k+1}) = y(x_k + h) = y_k + y'(x_k)h + \dfrac{1}{2} y''(x_k)h^2 + O(h^3)$

  and similarly: $y_{k-1} = y(x_{k-1}) = y(x_k - h) = y_k - y'(x_k)h + \dfrac{1}{2} y''(x_k)h^2 + O(h^3)$

Second-order derivative:

- Central scheme: $\boxed{y''(x_k) \sim \dfrac{y_{k-1} - 2y_k + y_{k+1}}{h^2}}$ Error: $O(h^2)$,

  since from Taylor's formula:

  $$y_{k+1} = y(x_{k+1}) = y(x_k + h) = y_k + y'(x_k)h + \frac{1}{2}y''(x_k)h^2 + \frac{1}{6}y'''(x_k)h^3 + O(h^4)$$

  $$y_{k-1} = y(x_{k-1}) = y(x_k - h) = y_k - y'(x_k)h + \frac{1}{2}y''(x_k)h^2 - \frac{1}{6}y'''(x_k)h^3 + O(h^4)$$

  Adding the two equalities, we have the proposition.

2. Approximation of the derivatives by integrating the differential equation

$$y(x_{k+1}) - y(x_k) = \int_{x_k}^{x_{k+1}} f(x, y(x))\, dx \;,$$

and by approximating the integral on the right-hand side by a proper quadrature formula:

Example (utilizing the trapezoidal rule): $y_{k+1} - y_k = \dfrac{1}{2}(f(x_k, y_k) + f(x_{k+1}, y_{k+1}))$

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Euler's method

Model problem:

$$y'(x) = f(x, y(x)), \qquad (x_0 < x < x_0 + A)$$
$$y(x_0) = y_0 \qquad (\textit{initial condition})$$

Computational grid: equidistant, with stepsize h: $x_0, x_1, x_2, \ldots, x_N$.

The derivatives of the solution at the gridpoints are approximated by finite differences of first order.

Explicit scheme (using the forward scheme):

$$y'(x_k) \approx \frac{y_{k+1} - y_k}{h} := f(x_k, y_k) \quad \Rightarrow \quad y_{k+1} := y_k + h \cdot f(x_k, y_k) \qquad (k = 0,1,\ldots,N-1)$$

Implicit scheme (using the backward scheme):

$$y'(x_{k+1}) \approx \frac{y_{k+1} - y_k}{h} := f(x_{k+1}, y_{k+1}) \Rightarrow \quad y_{k+1} := y_k + h \cdot f(x_{k+1}, y_{k+1}) \qquad (k = 0,1,\ldots,N-1)$$

Consistency, stability, convergence

Local error terms: $g_i := \dfrac{y(x_{i+1}) - y(x_i)}{h} - f(x_i, y(x_i)) \qquad (i = 0,1,\ldots,N-1)$

A method is said to be ***consistent in pth order***, if $g_i = O(h^p)$ (independently of i).

Global error terms: $e_i := y(x_i) - y_i \qquad (i = 0,1,\ldots,N-1)$

A method is said to be ***convergent in pth order***, if $e_i = O(h^p)$ (independently of i).

A method is said to be ***stable***, if the global error can be estimated by the local errors from above:

$$|e_i| \le C \cdot \left(|e_0| + h \sum_{j=0}^{i-1} |g_j| \right) \qquad (i = 0,1,\ldots,N-1)$$

If a method is consistent in pth order and stable, then it is also convergent in pth order.

Euler's method is convergent in first order.

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Improvements of Euler's method

Rewrite the original differential equation is the following form:

$$y(x_{k+1}) - y(x_k) = \int_{x_k}^{x_{k+1}} f(x, y(x))\, dx$$

Trapezoidal rule: Using the formula $\int_a^b F(x)dx \approx (b-a) \cdot \frac{F(a)+F(b)}{2}$, we have:

$$y_{k+1} := y_k + \frac{h}{2}\left(f(x_k, y_k) + f(x_{k+1}, y_k + hf(x_k, y_k)) \right)$$

In another form:

$$y_{k+1}^{*} := y_k + h \cdot f(x_k, y_k)$$
$$y_{k+1} := y_k + \frac{h}{2}\left(f(x_k, y_k) + f(x_{k+1}, y_{k+1}^{*}) \right)$$

The method is consistent in *second order*.

Midpoint rule: Using the formula $\int_a^b F(x)dx \approx (b-a)\cdot F\left(\frac{a+b}{2}\right)$, we have:

$$y_{k+1} := y_k + hf(x_{k+1/2}, y_k + \frac{h}{2} f(x_k, y_k))$$

In another form:

$$y_{k+1/2} := y_k + \frac{h}{2}\cdot f(x_k, y_k)$$
$$y_{k+1} := y_k + hf(x_{k+1/2}, y_{k+1/2})$$

The method is consistent in *second order*.

Conservation of the asymptotic stability

Consider the model problem

$$y' = -Ay$$

(with some $A > 0$). The identically zero function is an *asymptotically stable* solution of it, i.e. for every solution *y*, the equality $\lim_{x \to +\infty} y(x) = 0$ is valid, since $y(x) = y(0) \cdot e^{-Ax}$.

Now suppose that *h* is fixed, and investigate the validity of the limit $y_k \to 0$ for the values of the approximate solution at the gridpoints.

Explicit Euler method: $\qquad y_{k+1} := y_k - Ahy_k$

The asymptotic stability is not inherited for every *h* (**conditional stability**), since

$$y_k = y_{k-1} - Ahy_{k-1} = (1 - Ah)y_{k-1} = (1 - Ah)^2 y_{k-2} = \ldots = (1 - Ah)^k y_0 .$$

Thus $y_k \to 0$ for every y_0, if $|1 - Ah| < 1$, i.e. $-1 < 1 - Ah < 1$. This means that the asymptotic stability is inherited only if

$$\boxed{0 < h < \frac{2}{A}}$$

Implicit Euler method: $y_{k+1} := y_k - Ahy_{k+1}$

The asymptotic stability is now inherited for every h (**unconditional stability**), since $y_k := y_{k-1} - Ahy_k$ implies that:

$$\boxed{y_k = \frac{1}{1+Ah} y_{k-1} = \frac{1}{(1+Ah)^2} y_{k-2} = \ldots = \frac{1}{(1+Ah)^k} y_0}$$

Therefore $y_k \to 0$ is valid for every (positive) stepsize h.

Conservation of positivity

Consider the model problem

$$y' = -Ay$$

(with some $A > 0$). If the initial value is positive then the solution *y* is positive *everywhere*, since $y(x) = y(0) \cdot e^{-Ax}$.

Now suppose that *h* is fixed, and investigate the validity of the inequality $y_k > 0$ for the values of the approximate solution at the gridpoints provided that $y_0 > 0$.

Explicit Euler method: $$y_{k+1} := y_k - Ahy_k$$

The positivity is not preserved for every *h*, since

$$y_k = y_{k-1} - Ahy_{k-1} = (1 - Ah)y_{k-1} = (1 - Ah)^2 y_{k-2} = \ldots = (1 - Ah)^k y_0.$$

Thus, $y_k > 0$ for every $y_0 > 0$, if $0 < 1 - Ah < 1$. This means that the positivity is preserved only if

$$\boxed{0 < h < \frac{1}{A}}$$

Implicit Euler method: $$y_{k+1} := y_k - Ahy_{k+1}$$

Not the positivity is preserved for every positive stepsize *h*, since $y_k := y_{k-1} - Ahy_k$ implies that:

$$\boxed{y_k = \frac{1}{1+Ah} y_{k-1} = \frac{1}{(1+Ah)^2} y_{k-2} = \ldots = \frac{1}{(1+Ah)^k} y_0}$$

Therefore $y_k > 0$ is valid for every (positive) stepsize *h*.

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$$
\begin{aligned}
&k_1 := f(x_i, y_i) \\
&k_2 := f(x_i + h\cdot a_2, y_i + h\cdot b_{21}k_1) \\
&k_3 := f(x_i + h\cdot a_3, y_i + h\cdot b_{31}k_1 + h\cdot b_{32}k_2) \\
&\ldots \\
&k_s := f(x_i + h\cdot a_s, y_i + h\cdot b_{s1}k_1 + h\cdot b_{s2}k_2 + \ldots + h\cdot b_{s,s-1}k_{s-1}) \\
&y_{i+1} := y_i + h\cdot(c_1k_1 + c_2k_2 + \ldots + c_sk_s)
\end{aligned}
$$

A concrete method is characterized by the following parameters:

$$
\begin{aligned}
&s \\
&a_2, a_3, \ldots, a_s \\
&b_{21}; \quad b_{31}, b_{32}; \quad b_{41}, b_{42}, b_{43}; \quad \ldots \quad b_{s1}, b_{s2}, \ldots, b_{s,s-1} \\
&c_1, c_2, \ldots, c_s
\end{aligned}
$$

The parameters should be defined in such a way that the **local errors**, i.e. the numbers $\frac{y(x_{i+1}) - y(x_i)}{h} - \sum_{j=1}^{s} c_j k_j$ are of $O(h^p)$, where p is the **order** of the method.

Special Runge-Kutta methods

First order Runge-Kutta method: identical to the Euler method.

Second-order Runge-Kutta methods: the Euler method improved by the trapezoidal of the midpoint rule.

A third-order Runge-Kutta method:

$$k_1 := f(x_i, y_i), \qquad k_2 := f(x_i + \frac{h}{2}, y_i + \frac{h}{2} k_1), \qquad k_3 := f(x_i + h, y_i - h \cdot k_1 + 2h \cdot k_2)$$

$$y_{i+1} := y_i + \frac{h}{6} \cdot (k_1 + 4k_2 + k_3)$$

A fourth-order Runge-Kutta method:

$$k_1 := f(x_i, y_i), \qquad k_2 := f(x_i + \frac{h}{2}, y_i + \frac{h}{2} k_1),$$

$$k_3 := f(x_i + \frac{h}{2}, y_i + \frac{h}{2} k_2), \qquad k_4 := f(x_i + h, y_i + h \cdot k_3)$$

$$y_{i+1} := y_i + \frac{h}{6} \cdot (k_1 + 2k_2 + 2k_3 + k_4)$$

The order of the Runge-Kutta methods

For a given parameter *s*, the maximal order that can be achieved:

$$p = \begin{cases} = s & (s = 1,2,3,4) \\ \le s-1 & (s = 5,6,7) \\ \le s-2 & (s = 8,9) \\ \le s-3 & (s \ge 10) \end{cases}$$

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Linear multistep methods

The general form of the linear *k*-step methods is as follows:

$$\sum_{j=0}^{k} \alpha_j y_{i+j} = h \sum_{j=0}^{k} \beta_j f(x_{i+j}, y_{i+j}) \qquad (i = 0,1,\ldots,N-k)$$

The value y_0 is defined by the initial condition, while the values $y_1, y_2, \ldots, y_{k-1}$ should be defined by a completely different method (e.g. by a Runge-Kutta method). This is the task of the so-called **starting procedure**.

A concrete method is defined by the following parameters:

$$k, \quad \alpha_0, \alpha_1, \ldots, \alpha_k, \quad \beta_0, \beta_1, \ldots, \beta_k \qquad (\text{where } \alpha_k \neq 0),$$

Define the polynomials which characterize the method:

$$\rho(z) := \sum_{j=0}^{k} \alpha_j z^j, \qquad \sigma(z) := \sum_{j=0}^{k} \beta_j z^j$$

Consistency

The parameters should be defined in such a way that the **local errors** i.e. the numbers

$$g_i := \frac{1}{h}\sum_{j=0}^{k}\alpha_j y(x_{i+j}) - \sum_{j=0}^{k}\beta_j f(x_{i+j}, y(x_{i+j}))$$

are of order $O(h^p)$, where p is the **order** of the method.

The order of the method is (at least) p, if one of the conditions is satisfied:

(a) $C_0 = C_1 = C_2 = \ldots = C_p = 0$,

where $C_0 := \sum_{j=0}^{k}\alpha_j$, $C_1 := \frac{1}{1!}\sum_{j=0}^{k} j\alpha_j - \frac{1}{0!}\sum_{j=0}^{k}\beta_j$, $C_2 := \frac{1}{2!}\sum_{j=0}^{k} j^2\alpha_j - \frac{1}{1!}\sum_{j=0}^{k} j\beta_j, \ldots,$

$$C_p := \frac{1}{p!}\sum_{j=0}^{k} j^p\alpha_j - \frac{1}{(p-1)!}\sum_{j=0}^{k} j^{p-1}\beta_j \quad (\textit{error constants})$$

(b) the rational function $\rho(z)/\sigma(z)$ approximates the complex logarithm function in (p +1)th order around the point $z = 1$, i.e. $\frac{\rho(z)}{\sigma(z)} = \log z + O((z-1)^{p+1})$.

Stability and convergence

The method is said to be stable, if the polynomial ρ satisfies the *root condition*, i.e.
if the absolute values of its roots are at most 1,
and the roots whose absolute values equal to 1, are single roots (with multiplicity 1).

In this case, if the order of the method is p, then the method is convergent in pth order.

If the polynomial ρ satisfies the root condition, then the maximal order of consistency that can be achieved:

$p \le k+2$ if k is even, and $p \le k+1$, if k is odd. (*Dahlquist's theorem*)

Linear *k*-step methods of Adams type:

$$\rho(z) = z^k - z^{k-1}$$

Explicit methods of order k (Adams-Bashforth methods):

$k = 1$:

$$y_{i+1} := y_i + h \cdot f(x_i, y_i)$$

$k = 2$:

$$y_{i+1} := y_i + \frac{h}{2}(3f(x_i, y_i) - f(x_{i-1}, y_{i-1}))$$

$k = 3$:

$$y_{i+1} := y_i + \frac{h}{12}(23f(x_i, y_i) - 16f(x_{i-1}, y_{i-1}) + 5f(x_{i-2}, y_{i-2}))$$

$k = 4$:

$$y_{i+1} := y_i + \frac{h}{24}(55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2}) - 9f(x_{i-3}, y_{i-3}))$$

Linear *k*-step methods of Adams type:

$$\rho(z) = z^k - z^{k-1}$$

Implicit methods of order (k+1*)* (Adams-Moulton methods):

$k = 1$:

$$y_{i+1} := y_i + \frac{h}{2}(f(x_{i+1}, y_{i+1}) + f(x_i, y_i))$$

$k = 2$:

$$y_{i+1} := y_i + \frac{h}{12}(5f(x_{i+1}, y_{i+1}) + 8f(x_i, y_i) - f(x_{i-1}, y_{i-1}))$$

$k = 3$:

$$y_{i+1} := y_i + \frac{h}{24}(9f(x_{i+1}, y_{i+1}) + 19f(x_i, y_i) - 5f(x_{i-1}, y_{i-1}) + f(x_{i-2}, y_{i-2}))$$

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A model problem: Let σ be a given, positive function, and let q be a nonnegative function:

$$-(\sigma(x)u'(x))' + q(x)u(x) = f(x), \qquad (0 < x < 1)$$
$$u(0) = a, \quad u(1) = b$$

Computational grid: $x_k := kh \quad (k = 0,1,\ldots,N)$, where h is the stepsize: $h := 1/N$. The second-order term is approximated by a central scheme:

$$(\sigma u')'(x_k) \sim \frac{1}{h}\left(\sigma_{k+1}\frac{u_{k+1} - u_k}{h} - \sigma_k \frac{u_k - u_{k-1}}{h}\right) = \frac{1}{h^2}\left(\sigma_{k+1}u_{k+1} - (\sigma_{k+1} + \sigma_k)u_k + \sigma_{k-1}u_{k-1}\right)$$

u_0, u_N are predefined. The remaining u_k's can be computed by solving a linear system of equations:

$$-\sigma_{k-1}u_{k-1} + (\sigma_{k+1} + \sigma_k + h^2 q_k)u_k - \sigma_{k+1}u_{k+1} = h^2 f_k \qquad (k = 1,2,\ldots,N-1)$$

The matrix of the system is tridiagonal (moreover, it is diagonally dominant is each q_k is positive), thus, the solution can be performed in a computationally economic way (by $O(N)$ algebraic operations).