Mathematical modeling and numerical methods

Methods

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Contents

1 Analytical methods

1.1 Methods for first order ODE's

1.1.1 Separation of variables

An ODE which can be written on the form

$$g(y(x))y'(x) = f(x)$$

can be solved by finding the following integrals:

$$\int g(y)\,\mathrm{d}y = \int f(x)\,\mathrm{d}x + k,$$

and isolating y in the expression you get.

1.1.2 Exact ODE's

An ODE which can be written on the form

$$M(x, y(x)) + N(x, y(x))y'(x) = 0,$$

where N and M satisfy

$$\frac{\partial M}{\partial y}(x, y) = \frac{\partial N}{\partial x}(x, y),$$

can be solved by finding a function u of two variables which satisfies that

$$\frac{\partial u}{\partial x}(x, y) = M(x, y) \quad \text{and} \quad \frac{\partial u}{\partial y}(x, y) = N(x, y).$$

The function u can be found by first integrating M wrt. the first variable:

$$f(\cdot, y) = \int M(t, y)\,\mathrm{d}t,$$

and then defining

$$g(y) = N(x,y) - \frac{\partial f}{\partial y}(x,y),$$

(note that g turns out only to depend on one variable). Then u is given by

$$u(x,\cdot) = f(x,\cdot) + \int g(t)\,\mathrm{d}t.$$

Note that all antiderivatives are functions of an (unnamed) variable, which is represented by a dot ($\cdot$) wherever it appears in a given equation except in the antiderivates.

1.1.3 Integrating factors

Some ODE's which aren't exact can be transformed to exact ODE's by multiplying both sides with an *integrating factor*. In some instances, the following result can be used to finding an integrating factor.

Sætning 1.1. *If the functions P and Q in the ODE*

$$P(x,y(x)) + Q(x,y(x))y'(x) = 0$$

satisfy that

$$R(x,y) = \frac{1}{Q(x,y)}\Big(\frac{\partial P}{\partial y}(x,y) - \frac{\partial Q}{\partial x}(x,y)\Big)$$

is constant as a function of y for fixed x, then

$$F(x,y) = F(x) = \exp\int^x R(x_1,y)\,\mathrm{d}x_1$$

is an integrating factor. Correspondingly, if

$$R^*(x,y) = \frac{1}{P(x,y)}\Big(\frac{\partial Q}{\partial x}(x,y) - \frac{\partial P}{\partial y}(x,y)\Big)$$

is constant as function of x for fixed y, then

$$F^*(x,y) = F^*(y) = \exp\int^y R^*(x,y_1)\,\mathrm{d}y_1$$

is an integrating factor.

1.1.4 Homogeneous linear ODE's

For all numbers c,

$$y = ce^{-\int p(x)\,\mathrm{d}x}$$

is a solution to ODE's which can be written on the form

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

1.1.5 Inhomogeneous linear ODE's

An ODE which can be written on the form

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

has the following solutions:

$$y = e^{-h}\Big(\int e^{h(x)}r(x)\,\mathrm{d}x + c\Big), \quad \text{where} \quad h = \int p(x)\,\mathrm{d}x \quad \text{and} \quad c \in \mathbb{R}.$$

1.1.6 The Bernoulli equation

An ODE which can be written on the form

$$y'(x) + p(x)y(x) = g(x)y(x)^a,$$

where $a \neq 1$, can be solved by first finding a solution u to the following linear first order ODE:

$$u'(x) + (1-a)p(x)u(x) = (1-a)g(x),$$

and then setting

$$y(x) = u(x)^{\frac{1}{1-a}}.$$

1.2 Methods for second order ODE's

1.2.1 Homogeneous linear ODE's

1.2.1.1 Linearity of solutions/the superpositionprinciple

If y_1 and y_2 are defined on the same interval and both are solutions to the ODE

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0, \tag{1}$$

then $y = ay_1 + by_2$ is also a solution for all choices of real numbers $a, b \in \mathbb{R}$. The solutions y_1 and y_2 are linearly independent if and only if the Wronski determinant $W(y_1,y_2)(x) = y_1(x)y_2'(x) - y_2(x)y_1(x)$ is different from 0 for one (and hence all) x. If p and q are continuous and y_1 and y_2 er linearly independent, then all solutions are of the form $y = ay_1 + by_2$ and an initial value problem (1) with

$$y(x_0) = K_0, \qquad y'(x_0) = K_1$$

has a unique solution.

1.2.1.2 Reduction of order

Assume that y_1 is a solution to the ODE

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

then

$$y_2 = y_1 u, \quad \text{where} \quad u = \int v_1(x)\,\mathrm{d}x, \quad \text{and} \quad v_1 = \frac{1}{y_1^2} e^{-\int p(x)\,\mathrm{d}x}$$

is also a solution, and y_1 and y_2 are linearly independent.

Note that we don't care about the integration constants, as in one case it just corresponds to multiplying our solution with a positive number, and in the other case it corresponds to adding a constant factor of y_1.

1.2.1.3 Constant coefficients

The solutions to an ODE which can be written on the form

$$y''(x) + ay'(x) + by(x) = 0,$$

depends on the sign of the discriminant $a^2 - 4b$.

$a^2 - 4b > 0$: all solutions can be written on the form

$$y(x) = c_1 e^{\lambda_+ x} + c_2 e^{\lambda_- x},$$

where $\lambda_\pm = \frac{-a \pm \sqrt{a^2 - 4b}}{2}$ and $c_1, c_2 \in \mathbb{R}$.

$a^2 - 4b = 0$: all solutions can be written on the form

$$y(x) = c_1 e^{\lambda_0 x} + c_2 x e^{\lambda_0 x},$$

where $\lambda_0 = -\frac{a}{2}$ and $c_1, c_2 \in \mathbb{R}$.

$a^2 - 4b < 0$: all solutions can be written on the form

$$y(x) = c_1 e^{-\frac{ax}{2}} \sin(\omega x) + c_2 e^{-\frac{ax}{2}} \cos(\omega x),$$

where $\omega = \sqrt{b - \frac{1}{4}a^2}$.

1.2.1.4 Euler-Cauchy equations

The solutions to an ODE which can be written on the form

$$x^2 y''(x) + axy'(x) + by(x) = 0,$$

depends on the sign of the discriminant $(a-1)^2 - 4b$.

$(a-1)^2 - 4b > 0$: all solutions can be written on the form

$$y(x) = c_1 x^{m_+} + c_2 x^{m_-},$$

where $m_\pm = \frac{1-a}{2} \pm \sqrt{\frac{1}{4}(a-1)^2 - b}$ and $c_1, c_2 \in \mathbb{R}$.

$(a-1)^2 - 4b = 0$: all solutions can be written on the form

$$y(x) = c_1 x^{\frac{1-a}{2}} + c_2 \ln(|x|) x^{\frac{1-a}{2}}.$$

$(a-1)^2 - 4b < 0$: all solutions can be written on the form

$$y(x) = c_1 x^{\frac{1-a}{2}} \sin(\omega \ln(x)) + c_2 x^{\frac{1-a}{2}} \cos(\omega \ln(x)),$$

where $\omega = \sqrt{b - \frac{1}{4}(a-1)^2}$.

1.2.2 Non-homogeneous linear ODE's

1.2.2.1 Linearity of solutions/the superposition principle

The set of solutions of an ODE which can be written on the form

$$y''(x) + p(x)y'(x) + q(x)y(x) = r(x) \tag{2}$$

where $r \not\equiv 0$, is *not* linear, but if y_p is a solution to (2) (a *particular* solution), then any solution can be written on the form

$$y_g = y_p + y_h,$$

where y_h is a solution to the corresponding homogeneous equation

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0, \tag{3}$$

whose set of solutions is a linear space. Correspondingly, if y_p and $\tilde{y}_p$ are two solutions to (2), then $y_h = y_p - \tilde{y}_p$ is a solution to (3).

1.2.2.2 The method of undetermined coefficients

This method works by making a qualified guess y_p on a solution to an ODE which can be written on the form

$$y''(x) + ay'(x) + by(x) = r(x), \tag{4}$$

where a and b are constants, while $r = \sum_i r_i$ is a sum of functions which can be written in one of the following ways: $ke^{\gamma x}$, kx^n, $k\sin(\omega x)$, $k\cos(\omega x)$, $ke^{\alpha x}\sin(\omega x)$, $ke^{\alpha x}\cos(\omega x)$. Here, k, γ, and ω are real constants, while $n \in \mathbb{N} \cup \{0\}$. The qualified guess y_p has a term f_i per term r_i appearing in the sum $r = \sum_i r_i$, and these terms are chosen according to the following table.

Term r_i in $r(x)$	Choice of term f_i in $y_p(x)$
$ke^{\gamma x}$	$Ce^{\gamma x}$
kx^n ($n \in \mathbb{N}$)	$K_n x^n + K_{n-1}x^{n-1} + \cdots + K_1 x^1 + K_0$
$k\sin(\omega x)$, $k\cos(\omega x)$	$K\cos(\omega x) + M\sin(\omega x)$
$ke^{\alpha x}\cos(\omega x)$, $ke^{\alpha x}\sin(\omega x)$	$e^{\alpha x}(K\cos(\omega x) + M\sin(\omega x))$

Here, the constants γ, n, ω, and α are the same as in the corresponding term in r, while C, K, M, and K_j, $j = 0, \ldots, n$ are unknown constants for each term in $y_p = \sum f_i$, and which must be determined. If a term f_i is a solution to the corresponding homogeneous ODE,

$$y''(x) + ay'(x) + by(x) = 0, \tag{5}$$

then f_i is replaced by the function $\tilde{f}_i \colon x \mapsto xf_i$. If also $\tilde{f}_i$ is a solution to (5), then f_i is replaced by $x \mapsto x^2 f_i = x\tilde{f}_i$. The guess y_p is now plugged into the equation (4) and the unknown constants are determined.

1.2.2.3 Disturbed mass-spring systems

Consider the ODE

$$my''(t) + cy'(t) + ky(t) = F_0 \cos(\omega t),$$

where m, k, F_0, and ω are positive constants while c is non-negative and let $\omega_0 = \sqrt{\frac{k}{m}}$. If $c > 0$ or $\omega \neq \omega_0$, then

$$y_p(t) = a\cos(\omega t) + b\sin(\omega t) = C\cos(\omega t + \delta)$$

is a solution if $a = F_0 \dfrac{m(\omega_0^2 - \omega^2)}{m^2(\omega_0^2 - \omega^2)^2 + \omega^2 c^2}$ and $b = F_0 \dfrac{\omega c}{m^2(\omega_0^2 - \omega^2)^2 + \omega^2 c^2}$ or $\tan(\delta) = \frac{\omega c}{m(\omega_0^2 - \omega^2)}$ and $C = \frac{F_0}{\sqrt{m^2(\omega_0^2-\omega^2)^2+\omega^2c^2}}$.

If $c = 0$ and $\omega \neq \omega_0$, then it reduces to

$$y_p(t) = \frac{F_0}{m(\omega_0^2 - \omega^2)} \cos(\omega t)$$

and $\rho = \frac{k}{F_0} a = \frac{1}{1 - (\frac{\omega}{\omega_0})^2}$ is called the *resonance factor*. Another solution for $c = 0$ and $\omega \neq \omega_0$ is

$$\tilde{y}_p(t) = \frac{F_0}{m(\omega_0^2 - \omega^2)} \sin\left(\tfrac{\omega_0 + \omega}{2} t\right) \sin\left(\tfrac{\omega_0 - \omega}{2}\right).$$

If $c = 0$ and $\omega = \omega_0$ then

$$y_p(t) = \frac{F_0}{2m\omega_0} t$$

is a solution.

If $0 < c^2 \leq 2mk$, then the solutions have the biggest amplitude when $\omega = \sqrt{\omega_0^2 - \frac{c^2}{2m^2}}$ and in that case, all solutions tend to

$$y_p(t) = \frac{2mF_0}{c\sqrt{4m^2\omega_0^2 - c^2}} \cos(\omega t - \delta),$$

where $\tan(\delta) = \frac{2m\omega}{c}$ when $t \to \infty$.

1.2.2.4 Variation of parameters

An ODE which can be written on the form

$$y''(x) + p(x)y'(x) + q(x)y(x) = r(x),$$

where p, q, and r are continuous functions, has the solution

$$y_p = -y_1 \int \frac{y_2(x)r(x)}{W(x)} \, \mathrm{d}x + y_2 \int \frac{y_1(x)r(x)}{W(x)} \, \mathrm{d}x,$$

where y_1 and y_2 are solutions to the corresponding homogeneous problem,

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

and $W = y_1 y_2' - y_1' y_2$.

1.3 The Laplace transform

1.3.1 The Laplace transform of certain functions

$f(t)$	1	t	t^2	t^n $_{n=0,1,2,\ldots}$	t^a $_{a\geq 0}$	e^{at}
$\mathcal{L}(f)(s)$	$\frac{1}{s}$	$\frac{1}{s^2}$	$\frac{2!}{s^3}$	$\frac{n!}{s^{n+1}}$	$\frac{\Gamma(a+1)}{s^{a+1}}$	$\frac{1}{s-a}$

$f(t)$	$\cos(\omega t)$	$\sin(\omega t)$	$\cosh(at)$	$\sinh(at)$	$e^{at}\cos(\omega t)$	$e^{at}\sin(\omega t)$
$\mathcal{L}(f)(s)$	$\frac{s}{s^2+\omega^2}$	$\frac{\omega}{s^2+\omega^2}$	$\frac{s}{s^2-a^2}$	$\frac{a}{s^2-a^2}$	$\frac{s-a}{(s-a)^2+\omega^2}$	$\frac{\omega}{(s-a)^2+\omega^2}$

1.3.2 Linearity of the Laplace transform and its inverse

the Laplace transform is linear, i.e. if one knows the Laplace transform $\mathcal{L}(f)$ of f and the Laplace transform $\mathcal{L}(g)$ of g, then one can compute the Laplace transform of $af + bg$, where a and b are real numbers, in the following way:

$$\mathcal{L}(af + bg) = a\mathcal{L}(f) + b\mathcal{L}(g).$$

Likewise, the inverse of the Laplace transform is linear, i.e. if one knows $\mathcal{L}^{-1}(F) = f$ and $\mathcal{L}^{-1}(G) = g$, then one can compute the inverse Laplace transform of $aF+bG$, where a and b are real numbers, in the following way:

$$\mathcal{L}^{-1}(aF + bG) = a\mathcal{L}^{-1}(F) + b\mathcal{L}^{-1}(G).$$

1.3.3 s-shifting

If $\mathcal{L}(f) = F$, and $g(t) = e^{at}f(t)$, then $\mathcal{L}(g)(s) = \mathcal{L}(t \mapsto e^{at}f(t))(s) = F(s - a)$.

1.3.4 the Laplace transform of derivatives

If the Laplace transform $F = \mathcal{L}(f)$ of f and the derivative of f exist, then

$$\mathcal{L}(f^{(n)})(s) = s^nF(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - s^1f^{(n-2)}(0) - f^{(n-1)}(0).$$

In particular

$$\mathcal{L}(f'')(s) = s^2F(s) - sf(0) - f'(0)$$

and

$$\mathcal{L}(f')(s) = sF(s) - f(0).$$

1.3.5 the Laplace transform of integrals

If the Laplace transform $\mathcal{L}(f) = F$ of f and the Laplace transform of the integral of f exist, i.e. if the Laplace transform $G = \mathcal{L}(g)$ of the function g given by $g(t) = \int_0^t f(x)\,\mathrm{d}x$ exists, then

$$G(s) = \mathcal{L}(g)(s) = \mathcal{L}(t \mapsto \int_0^t f(x)\,\mathrm{d}x)(s) = \frac{1}{s}F(s).$$

1.3.6 solution of initial value problems

1.3.6.1 initial value problems with $t_0 = 0$

Initial value problems such as

$$y''(t) + ay'(t) + by(t) = r(t), \quad y(0) = K_0, \quad y'(0) = K_1,$$

where a, b, K_0, and K_1 are constants, and the function r is sufficiently nice, can be rewritten to an algebraic problem by taking the Laplace transform on both sides:

$$\mathcal{L}(y'' + ay' + by)(s) = \mathcal{L}(r)(t)$$

which in this case can be written as

$$(s^2Y(s) - sy(0) - y'(0)) + a(sY(s) - y(0)) + bY(s) = (s^2 + as + b)Y(s) - (s + a)K_0 - K_1 = R(s)$$

where $Y = \mathcal{L}(y)$ and $R = \mathcal{L}(r)$. By isolating $Y(s)$ one gets

$$Y(s) = \frac{(s + a)K_0 + K_1 + R(s)}{s^2 + as + b} = \big((s + a)K_0 + K_1\big)Q(s) + R(s)Q(s), \tag{6}$$

where $Q(s) = \frac{1}{s^2+as+b} = \frac{1}{(s+\frac{1}{2}a)^2+b-\frac{1}{4}a^2}$. We can now solve the initial value problem by taking the inverse Laplace transform of $((s + a)K_0 + K_1)Q(s) + R(s)Q(s)$.

1.3.6.2 Shifted data problems

Initial value problems such as

$$y''(t) + ay'(t) + by(t) = r(t), \quad y(t_0) = K_0, \quad y'(t_0) = K_1,$$

where a, b, K_0, and K_1 are constants and $t_0 \neq 0$, can be solved by at setting $\tilde{t} = t - t_0$, $\tilde{y}(\tilde{t}) = y(\tilde{t} + t_0)$, and solving

$$\tilde{y}''(\tilde{t}) + a\tilde{y}'(\tilde{t}) + b\tilde{y}(\tilde{t}) = r(\tilde{t}), \quad \tilde{y}(0) = K_0, \quad \tilde{y}'(0) = K_1,$$

by finding $\tilde{Y}$ and then $\tilde{y}(\tilde{t})$, then y can be found by using that $y(t) = \tilde{y}(\tilde{t}) = \tilde{y}(t - t_0)$.

1.3.7 Partial fractions

assume that we have a polynomial fraction on the following form:

$$\frac{P(s)}{Q(s)},$$

where

$$Q(s) = \prod_{i=1}^{n}(s - r_i) \prod_{j=1}^{m}(s^2 + a_js + b_j), \quad \text{where} \quad r_i \leq r_{i+1}, a_j \leq a_{j+1},$$

and where $s^2 + a_js + b_j$ has no real roots for $j = 1, \ldots, m$, and $P(s)$ is a polynomial of degree $n + 2m - 1$ or degree $n + 2m - 2$. If $r_i \neq r_{i+1}$ for all $i = 1, \ldots, n - 1$, and $a_js + b_j \neq a_{j+1}s + b_{j+1}$ for all $j = 1, \dots, m-1$, and one can find $n+2m$ constants, $A_k, B_l, C_l, \in \mathbb{R}$, $k = 1, \dots, n$, $l = 1, \dots, m$, such that

$$P(s) = \sum_{k=1}^{n} A_k \prod_{\substack{i=1 \\ i\neq k}}^{n} (s - r_i) \prod_{j=1}^{m} (s^2 + a_j + b_j) + \sum_{l=1}^{m} (B_l s + C_l) \prod_{i=1}^{n} (s - r_i) \prod_{\substack{j=1 \\ j\neq l}}^{m} (s^2 + a_j s + b_j), \quad (7)$$

then

$$\frac{P(s)}{Q(s)} = \sum_{k=1}^{n} \frac{A_k}{s - r_k} + \sum_{l=1}^{m} \frac{B_k s + C_k}{s^2 + a_k s + b_k},$$

where we recall that $s^2 + a_k s + b_k = (s + \frac{1}{2}a_k)^2 + b_k - \frac{1}{4}a_k^2$. If in addition we have that $m = 0$, then the constants A_k can be found just by plugging r_k into (7) and isolating A_k:

$$A_k = \frac{P(r_k)}{\prod_{\substack{i=1 \\ i\neq k}}^{n} (r_k - r_i)} \qquad \text{(if } m = 0\text{)}.$$

If instead $r_i = r_{i+1}$ (but $r_{i+1} \neq r_{i+2}$, if $i \leq n-2$) for one or more $i \in \{1, 2, \dots, n-1\}$, and $a_j s + b_j \neq a_{j+1} s + b_{j+1}$ for all $j = 1, \dots, m-1$, and one can find $n + 2m$ constants, $A_k, B_l, C_l, \in \mathbb{R}$, $k = 1, \dots, n$, $l = 1, \dots, m$, such that

$$\begin{aligned} P(s) = A_1 \prod_{i=2}^{n} (s - r_i) \prod_{j=1}^{m} (s^2 + a_j + b_j) &+ \sum_{\substack{k=2 \\ r_k \neq r_{k-1}}}^{n} A_k \prod_{\substack{i=1 \\ i\neq k}}^{n} (s - r_i) \prod_{j=1}^{m} (s^2 + a_j s + b_j) \\ &+ \sum_{\substack{k=2 \\ r_k = r_{k-1}}}^{n} A_k (s - r_k) \prod_{\substack{i=1 \\ i\neq k}}^{n} (s - r_i) \prod_{j=1}^{m} (s^2 + a_j + b_j) \\ &+ \sum_{l=1}^{m} (B_l s + C_l) \prod_{i=1}^{n} (s - r_i) \prod_{\substack{j=1 \\ j\neq l}}^{m} (s^2 + a_j + b_j), \end{aligned} \quad (8)$$

then

$$\frac{P(s)}{Q(s)} = \frac{A_1}{s - r_1} + \sum_{\substack{k=2 \\ r_k \neq r_{k-1}}}^{n} \frac{A_k}{s - r_k} + \sum_{\substack{k=2 \\ r_k = r_{k-1}}}^{n} \frac{A_k}{(s - r_k)^2} + \sum_{l=1}^{m} \frac{B_k s + C_k}{s^2 + a_k s + b_k}. \quad (9)$$

Similar tricks work also in the case where $r_i = r_{i+1} = \cdots = r_{i+k}$ for $k \geq 2$ and one (or more) indices $i \in \{1, \dots, n-1\}$, or $a_j s + b_j = a_{j+1} s + b_{j+1}$ for some $j \in \{1, \dots, m-1\}$, but the formulas corresponding to (8) and (9) become correspondingly more complicated. In this case, it is recommended to proceed by trial and error with expressions similar to (9) and from this find an expression of the form (8) by multiplying with $Q(s)$ on both sides.

1.4 Systems of ODE's

1.4.1 Conversion of ODE's of order n to systems of n ODE's of order 1

An ODE of order n of the form

$$y^{(n)}(t) = F(t, y(t), y'(t), \dots, y^{(n-1)}(t))$$

is equivalent with the following system of n ODE's of first order:

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= y_3 \\ &\cdots \\ y_{n-1}' &= y_n \\ y_n' &= F(t,y_1,y_2,\dots,y_n) \end{aligned}$$

via the identification

$$y_1 = y, \quad y_2 = y', \quad y_3 = y'', \quad \cdots \quad y_n = y^{(n-1)}.$$

1.4.2 Systems of ODE's of order 1 with constant coefficient matrices

Et system of n ODE's of order 1 of the form

$$y' = Ay,$$

where A is a constant coefficient matrix with real eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ with corresponding eigenvectors $v_1, v_2, \dots, v_n$, has the general solution

$$c_1 v_1 e^{\lambda_1} + c_2 v_2 e^{\lambda_2} + \cdots + c_n v_n e^{\lambda_n},$$

where $c_1, c_2, \dots, c_n$ are real constants.

1.5 Fourier series

1.5.1 Computation of Fourier coefficients etc.

If f is a 2π-periodic function which is sufficiently nice, then the Fourier coefficients of f are given by

$$\begin{aligned} a_0(f) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\,\mathrm{d}x, \\ a_n(f) &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)\,\mathrm{d}x \quad \text{and} \\ b_n(f) &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)\,\mathrm{d}x \end{aligned}$$

for all $n \in \mathbb{N}$ and the Fourier series for f is given by

$$a_0(f) + \sum_{n=1}^{\infty}\big(a_n(f)\cos(nx) + b_n(f)\sin(nx)\big). \tag{10}$$

If f is piecewise continuous with left- and right-derivatives everywhere, then it is sufficiently nice in the above sense and the Fourier series (10) converges pointwise towards f in the continuity points of f, while it converges towards the average of the left and right limit at discontinuity points.

1.5.2 Even and odd functions

If f is 2π-periodic, sufficiently nice and even (i.e. $f(-x) = f(x)$), then $b_n(f) = 0$ for all $n \geq 1$ and $a_n(f)$, $n \geq 0$, can be computed in the following way:

$$a_0(f) = \frac{1}{\pi}\int_0^{\pi} f(x)\,\mathrm{d}x \quad \text{and} \quad a_n(f) = \frac{2}{\pi}\int_0^{\pi} f(x)\cos(nx)\,\mathrm{d}x \quad \text{for } n = 1,2,3,\dots .$$

If f is 2π-periodic, sufficiently nice and odd (i.e. $f(-x) = -f(x)$), then $a_n(f) = 0$ for all $n \geq 0$ and $b_n(f)$, $n \geq 1$, can be computed in the following way:

$$b_n(f) = \frac{2}{\pi}\int_0^{\pi} f(x)\sin(nx)\,\mathrm{d}x.$$

1.5.3 Linearity of Fourier coefficients

If f and g have the Fourier coefficients $a_0(f)$, $a_n(f)$, and $b_n(f)$ resp. $a_0(g)$, $a_n(g)$, and $b_n(g)$, then the function $c_1 f + c_2 g$, where c_1 and c_2 are real numbers, has the Fourier coefficients

$$\begin{aligned} a_0(c_1 f + c_2 g) &= c_1 a_0(f) + c_2 a_0(g), \\ a_n(c_1 f + c_2 g) &= c_1 a_n(f) + c_2 a_n(g) \quad \text{and} \\ b_n(c_1 f + c_2 g) &= c_1 b_n(f) + c_2 b_n(g), \end{aligned}$$

where $n = 1, 2, 3, \dots$.

1.5.4 Change of period

If f is $2L$-periodic, then the Fourier series for f is given by

$$a_0(f) + \sum_{n=1}^{\infty}\left(a_n(f)\cos\left(\frac{n\pi}{L}x\right) + b_n(f)\sin\left(\frac{n\pi}{L}x\right)\right),$$

where

$$\begin{aligned} a_0(f) &= \frac{1}{2L}\int_{-L}^{L} f(x)\,\mathrm{d}x \\ a_n(f) &= \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{n\pi}{L}x\right)\mathrm{d}x \\ b_n(f) &= \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{n\pi}{L}x\right)\mathrm{d}x, \end{aligned}$$

for $n = 1, 2, 3, \dots$.

1.5.5 Half-range expansions

If $f\colon [0, L] \to \mathbb{R}$ is continuous, then

$$f(x) = a_0(f) + \sum_{n=1}^{\infty} a_n(f)\cos\left(\frac{n\pi}{L}x\right) = \sum_{n=1}^{\infty} b_n(f)\sin\left(\frac{n\pi}{L}x\right)$$

for all $x \in (0, L)$, where

$$a_0(f) = \frac{1}{L}\int_0^L f(x)\,\mathrm{d}x$$
$$a_n(f) = \frac{2}{L}\int_0^L f(x)\cos\Big(\frac{n\pi}{L}x\Big)\,\mathrm{d}x \quad \text{and}$$
$$b_n(f) = \frac{2}{L}\int_0^L f(x)\sin\Big(\frac{n\pi}{L}x\Big)\,\mathrm{d}x.$$

The functions f_l and f_u defined for all $x \in \mathbb{R}$ and given by

$$f_l(x) = a_0(f) + \sum_{n=1}^{\infty} a_n(f)\cos\Big(\frac{n\pi}{L}x\Big) \quad \text{and} \quad f_u(x) = \sum_{n=1}^{\infty} b_n(f)\sin\Big(\frac{n\pi}{L}x\Big)$$

are resp. the even and the odd $2L$-periodic expansion of f.

1.6 Methods for second order PDE's

1.6.1 The one-dimensional wave equation

The one-dimensional wave equation

$$u_{tt} = c^2 u_{xx}, \quad \text{where} \quad c^2 = \frac{T}{\rho}, \tag{11}$$

on $(x, t) \in [0, L] \times \mathbb{R}_{\geq 0}$ with the boundary condition

$$u(0, t) = u(L, t) = 0 \tag{12}$$

and the initial value conditions

$$u(x, 0) = f(x) \tag{13}$$

and

$$u_t(x, 0) = g(x), \tag{14}$$

where $f, g\colon [0, L] \to \mathbb{R}$ are two sufficiently nice functions, can be solved as described in the following subsubsections.

1.6.1.1 The Fourier series method

Let $\lambda_n = \frac{cn\pi}{L}$ and

$$u(x, t) = \sum_{n=1}^{\infty} u_n(x, t) = \sum_{n=1}^{\infty}\big(b_n\cos(\lambda_n t) + b_n^*\sin(\lambda_n t)\big)\sin\Big(\frac{n\pi}{L}x\Big),$$

where the b_n's are the Fourier coefficients of the $2L$-periodic, odd, half-range expansion of f

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\Big(\frac{n\pi}{L}x\Big)\,\mathrm{d}x$$

and

$$b_n^* = \frac{2}{cn\pi} \int_0^L g(x) \sin\Big(\frac{n\pi}{L} x\Big) \,\mathrm{d}x.$$

then u is the solution to the wave equation (11) with the boundary condition (12) and the initial value conditions (13) and (14). The functions $u_n(x,t) = \big(b_n \cos(\lambda_n t) + b_n^* \sin(\lambda_n t)\big) \sin\big(\frac{n\pi}{L} x\big)$ are called *eigenfunctions* with *eigenvalues* λ_n and have the frequencies $\frac{\lambda_n}{2\pi}$. The set $\{\lambda_n \mid n \in \mathbb{N}\}$ is called the *spectrum*, u_1 is called the *fundamental mode*, while u_n are called *overtones* for $n \geq 1$.

1.6.1.2 D'Alembert's solution

Let

$$u(x,t) = \frac{1}{2}\big(f(x+ct) + f(x-ct)\big) + \frac{1}{2c} \int_{x-ct}^{x+ct} g(s) \,\mathrm{d}s,$$

where f and g are assumed to be odd and $2L$-periodic. then u is the solution to the wave equation (11) with the boundary condition (12) and the initial value conditions (13) and (14).

1.6.2 The one-dimensional heat equation

The solution to the one-dimensional heat equation

$$u_t = c^2 u_{xx}, \quad \text{where} \quad c^2 = \frac{K}{\sigma\rho}, \tag{15}$$

on $(x,t) \in [0,L] \times \mathbb{R}_{\geq 0}$ and the initial value condition

$$u(x,0) = f(x) \tag{16}$$

where $f\colon [0,L] \to \mathbb{R}$ is a sufficiently nice function, depends on the boundary condition as described in the the following subsubsections.

1.6.2.1 The boundary condition $u(0,t) = u(L,t) = 0$

If both ends are kept at the temperature 0, then the system has the boundary condition

$$u(0,t) = u(L,t) = 0. \tag{17}$$

If so,

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} b_n(f) \sin\Big(\frac{n\pi}{L} x\Big) e^{-\lambda_n^2 t},$$

where $\lambda_n = \frac{cn\pi}{L}$ and

$$b_n(f) = \frac{2}{L} \int_0^L f(x) \sin\Big(\frac{n\pi}{L} x\Big) \,\mathrm{d}x,$$

is the solution to (15) with the initial value condition (16) and the boundary conditions (17). The coefficients $b_n(f)$ are thus the Fourier coefficients of the $2L$-periodic, odd, half-range expansion of f. The functions $u_n(x,t) = \sin\big(\frac{n\pi}{L} x\big) e^{-\lambda_n^2 t}$ are called the *eigenfunctions* of the problem with *eigenvalues* λ_n.

1.6.2.2 Isolated endpoints

If both ends are isolated, then the system has the boundary condition

$$u_x(0,t) = u_x(L,t) = 0. \tag{18}$$

If so,

$$u(x,t) = \sum_{n=0}^{\infty} u_n(x,t) = a_0(f) + \sum_{n=1}^{\infty} a_n(f)\cos\Big(\frac{n\pi}{L}x\Big)e^{-\lambda_n^2 t},$$

where $\lambda_n = \frac{cn\pi}{L}$ and

$$a_0(f) = \frac{1}{L}\int_0^L f(x)\,\mathrm{d}x \quad \text{and} \quad a_n(f) = \frac{2}{L}\int_0^L f(x)\cos\Big(\frac{n\pi}{L}x\Big)\,\mathrm{d}x \quad \text{for} \quad n \geq 1,$$

is the solution to (15) with the initial value condition (16) and the boundary condition (18). The coefficients $a_0(f)$ and $a_n(f)$ are thus the Fourier coefficients of the $2L$-periodic, even, half-range expansion of f. The functions $u_n(x,t) = \sin\big(\frac{n\pi}{L}x\big)e^{-\lambda_n^2 t}$ are called the *eigenfunctions* of the problem with *eigenvalues* λ_n.

2 Numerical methods

2.1 solution of equations

2.1.1 Fixed-point iteration

Assume that we want to find a solution to an equation of the form

$$g(x) = x.$$

Let x_0 be a guess for a solution s to the equation $g(x) = x$. Now define recursively

$$x_1 = g(x_0), \quad x_2 = g(x_1), \quad \ldots, \quad x_{n+1} = g(x_n), \quad \ldots,$$

for all $n \geq 1$. In some cases the sequence $\{x_n\}_{n=0}^{\infty}$ will now approach the solution s when n grows, i.e. $x_n \to s$ for $n \to \infty$. A sufficient condition is given in the Theorem below.

Sætning 2.1. *Let s be a solution to $x = g(x)$ and assume that g is continuously differentiable in an interval J around s. If $|g'(x)| \leq K < 1$ i J, then the sequence converges $\{x_n\}_{n=0}^{\infty}$ towards $x_\infty = s$, whenever $x_0 \in J$.*

2.1.2 Newton's method

Assume that we want to find a solution to an equation of the form

$$f(x) = 0,$$

where f is a continuously differentiable function. Let x_0 be a guess for a solution s to the equation $f(x) = 0$. Now define recursively

$$x_1 = s_0 - \frac{f(x_0)}{f'(x_0)}, \quad x_2 = x_2 - \frac{f(x_1)}{f'(x_2)}, \quad \ldots, \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \quad \ldots,$$

for all $n \geq 1$. In some cases the sequence $\{x_n\}_{n=0}^{\infty}$ will now approach the solution s, when n grows, i.e. $x_n \to s$ for $n \to \infty$. The following Theorem gives information about hte rate of convergence.

Sætning 2.2. *If f is twice differentiable and $f'(s) \neq 0$, where $f(s) = 0$ is a solution, then Newton's method is at least of order 2.*

2.1.3 The secant method

Assume that we want to find a solution to an equation of the form

$$f(x) = 0.$$

Let x_0 and x_1 be two different guesses for a solution s to the equation $f(x) = 0$. Now define recursively

$$x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}, \qquad x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)},$$

$$\ldots$$

$$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})},$$

$$\ldots$$

for all $n \geq 1$. In some cases the sequence $\{x_n\}_{n=0}^{\infty}$ will now approach the solution s, when n grows, i.e. $x_n \to s$ for $n \to \infty$.

2.2 Interpolation polynomials

2.2.1 A polynomial through $n + 1$ points

Given $n + 1$ points in the plane, (x_i, y_i), $i = 0, \ldots, n$, where $x_i \neq x_i$ when $i \neq j$, there exists a unique polynomial p_n of degree (at most) n, such that $p_n(x_i) = y_i$.

2.2.1.1 Lagrange interpolation

Let (x_i, y_i), $i = 0, \ldots, n$ be $n + 1$ points in the plane where $x_i \neq x_j$ for $i \neq j$. Let

$$\ell_j(x) = \prod_{\substack{i=0 \\ i \neq j}}^{n} (x - x_i) = (x - x_0)(x - x_1) \cdots (x - x_{j-1})(x - x_{j+1}) \cdots (x - x_n)$$

and

$$L_j(x) = \frac{l_j(x)}{l_j(x_j)}.$$

then

$$p_n(x) = \sum_{i=0}^{n} y_i L_i(x)$$

is the polynomial of degree (at most) n, such that $p_n(x_i) = y_i$.

2.2.1.2 Newton's divided difference method

Let (x_i, y_i), $i = 0, \ldots, n$ be $n+1$ points in the plane where $x_i \neq x_j$ for $i \neq j$. Let

$$f[x_i] = y_i,$$

$$f[x_0, \ldots, x_k] = \frac{f[x_1, \ldots, x_k] - f[x_0, \ldots, x_{k-1}]}{x_k - x_0},$$

and

$$g_i(x) = f[x_0, \ldots, x_i](x - x_0) \cdots (x - x_{i-1}) = f[x_0, \ldots, x_i] \prod_{j<i} (x - x_j).$$

then

$$p_n(x) = \sum_{i=0}^{n} g_i(x)$$

is the polynomial of degree (at most) n, such that $p_n(x_i) = y_i$.

2.2.2 Polynomial approximation of functions

If $f\colon A \to \mathbb{R}$, $A \subset \mathbb{R}$ is a function which we know the values of at x_i, $i = 0, \ldots, n$, where $x_i \neq x_j$ for $i \neq j$, i.e. if ve know $f(x_i)$ for $i = 0, \ldots, n$, then polynomial p_n through $(x_i, f(x_i))$, $i = 0, \ldots, n$, is called a *polynomial approximation* of f. If $x \in [\min_i(x_i), \max_i(x_i)]$, then $p_n(x)$ is called the *interpolated value*, while $p_n(x)$ is called the *ekstrapolated value*, if $x \notin [\min_i(x_i), \max_i(x_i)]$. If we for a $x \in [\min_i(x_i), \max_i(x_i)]$ use $p_n(x)$ instead of $f(x)$, then the error

$$\varepsilon_n = f(x) - p_n(x) = (x - x_0)(x - x_1) \cdots (x - x_n) \frac{f^{(n+1)}(t_x)}{(n+1)!}$$

for some $t_x \in [\min_i(x_i), \max_i(x_i)]$. We can then find an upper and a lower bound for ε_n by finding upper and lower bounds for $f^{(n+1)}$.

2.3 Numerical integration

2.3.1 Rectangular rule

Let $f\colon [a, b] \to \mathbb{R}$. For a $n \in \mathbb{N}$ we put $h = \frac{b-a}{n}$ and $x_0 = a$, $x_i = x_0 + ih$ for $i = 1, \ldots, n$.. then

$$J_n^m = h \sum_{i=1}^{n} f(x_i - \tfrac{h}{2})$$

is an approximation of $\int_a^b f(x)\,\mathrm{d}x$ and if f is sufficiently nice – e.g. if f is continuous – then we have that $J_n^m \to \int_a^b f(x)\,\mathrm{d}x$ for $n \to \infty$. The rectangular rule has degree of precision 1.

2.3.2 The trapezoidal rule

Let $f\colon [a,b] \to \mathbb{R}$. For a $n \in \mathbb{N}$ we put $h = \frac{b-a}{n}$ and $x_0 = a$, $x_i = x_0 + ih$ for $i = 1, \dots, n$. Then

$$J_n^t = \frac{h}{2}\big(f(a) + f(b)\big) + h\sum_{i=1}^{n-1} f(x_i)$$

is an approximation of $\int_a^b f(x)\,\mathrm{d}x$ and if f is sufficiently nice – e.g. if f is continuous – then we have that $J_n^t \to \int_a^b f(x)\,\mathrm{d}x$ for $n \to \infty$. If f is twice differentiable, then there exists a $x_t \in [a,b]$ such that

$$\varepsilon_n^t = -\frac{b-a}{12} h^2 f''(x_t),$$

where $\varepsilon_n^t = \int_a^b f(x)\,\mathrm{d}x - J_n^t$ is the error in the approximation. If n is an even number, the error can be approximated via the following formula:

$$\varepsilon_n^t \approx \frac{1}{3}(J_n^t - J_{\frac{n}{2}}^t).$$

The trapezoidal rule has degree of precision 1.

2.3.3 Simpson's rule

Let $f\colon [a,b] \to \mathbb{R}$. For a $n \in \mathbb{N}$ we put $h = \frac{b-a}{n}$ and $x_0 = a$, $x_i = x_0 + ih$ for $i = 1, \dots, n$. Then

$$J_n^S = \frac{h}{6}\big(f(a) + f(b)\big) + \frac{2h}{3}\sum_{i=1}^{n} f(x_i - \tfrac{h}{2}) + \frac{h}{3}\sum_{i=1}^{n-1} f(x_i)$$

is an approximation of $\int_a^b f(x)\,\mathrm{d}x$ and if f is sufficiently nice – e.g. if f is continuous – then we have that $J_n^S \to \int_a^b f(x)\,\mathrm{d}x$ for $n \to \infty$. If f is four times differentiable, then there exists a $x_S \in [a,b]$ then

$$\varepsilon_n^S = -\frac{(b-a)}{2880} h^4 f^{(4)}(x_S),$$

where $\varepsilon_n^S = \int_a^b f(x)\,\mathrm{d}x - J_n^S$ is the error in the approximation. If n is an even number, the error can be approksimated via the following formula:

$$\varepsilon_n^S \approx \frac{1}{15}(J_n^S - J_{\frac{n}{2}}^S).$$

Simpson's rule has degree of precision 3.

2.3.4 Gauss integration

Let $f\colon [a,b] \to \mathbb{R}$. For a $n \in \mathbb{N}$, $n \geq 2$, we put

$$J_n^G = \frac{b-a}{2}\sum_{i=1}^{n} w_i f\Big(\frac{b-a}{2} z_i + \frac{a+b}{2}\Big),$$

for some particular weights w_i and points z_i. For n between 2 and 5 the weights and points can be found in the following table.

Number of points n	points z_i	weights w_i	degree of precision N
2	$\pm\frac{\sqrt{3}}{3}$	1	3
3	0 $\pm\sqrt{\frac{3}{5}}$	$\frac{8}{9}$ $\frac{5}{9}$	5
4	$\pm\sqrt{\frac{3-2\sqrt{\frac{6}{5}}}{7}}$ $\pm\sqrt{\frac{3+2\sqrt{\frac{6}{5}}}{7}}$	$\frac{18+\sqrt{30}}{36}$ $\frac{18-\sqrt{30}}{36}$	7
5	0 $\pm\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$ $\pm\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	$\frac{128}{225}$ $\frac{322+13\sqrt{70}}{900}$ $\frac{322-13\sqrt{70}}{900}$	9

Gauss integration has degree of precision $2n-1$.

2.4 One-step methods for numerical solution of first order ODE's

In numerical one-step methods for solution of first order ODE's, one finds sequences x_n and y_n, with $x_n < x_{n+1}$, such that $y(x_n) \approx y_n$, where y_n is found using x_{n-1} and y_{n-1}.

2.4.1 The Euler method

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n, $n = 0, 1, 2, \ldots$, recursively by

$$y_{n+1} = y_n + hf(x_n, y_n).$$

then the local truncation error is $O(h^2)$ and the global truncation error is $O(h)$. The Euler method is thus a first order method.

2.4.2 Heun's method

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n, $n = 0, 1, 2, \ldots$, recursively by

$$\tilde{y}_{n+1} = y_n + hf(x_n, y_n)$$

and

$$y_{n+1} = y_n + \frac{h}{2}\big(f(x_n, y_n) + f(x_{n+1}, \tilde{y}_{n+1})\big).$$

Heun's method is a second order method with local truncation error $O(h^3)$ and global truncation error $O(h^2)$.

2.4.3 The RK4 method

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n, $n = 0, 1, 2, \ldots$, recursively by

$$y_{n+1} = y_n + \frac{1}{6}\big(k_1 + 2k_2 + 2k_3 + k_4\big), \qquad \text{for} \qquad n = 0,1,2,\ldots,$$

where

$$\begin{aligned} k_1 &= hf(x_n, y_n), \\ k_2 &= hf(x_n + \tfrac{h}{2}, y_n + \tfrac{1}{2}k_1), \\ k_3 &= hf(x_n + \tfrac{h}{2}, y_n + \tfrac{1}{2}k_2), \\ k_4 &= hf(x_n + h, y_n + k_3). \end{aligned}$$

The RK4 method is a fourth order method with local truncation error $O(h^5)$ and global truncation error $O(h^4)$. The error $\varepsilon^h_{2n} = y(x_{2n}) - y_{2n}$ can be estimated by

$$\varepsilon^h_{2n} \approx \frac{1}{15}(y^h_{2n} - y^{2h}_n).$$

2.4.4 Runge-Kutta-Fehlberg

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n, $n = 0, 1, 2, \ldots$, recursively by

$$y_{n+1} = y_n + \gamma_1 k_1 + \cdots + \gamma_6 k_6$$

and

$$\tilde{y}_{n+1} = y_n + \tilde{\gamma}_1 k_1 + \cdots + \tilde{\gamma}_5 k_5,$$

where

$$\begin{pmatrix}\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_5 & \gamma_6\end{pmatrix} = \begin{pmatrix}\frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & \frac{-9}{50} & \frac{2}{55}\end{pmatrix}$$

and

$$\begin{pmatrix}\tilde{\gamma}_1 & \tilde{\gamma}_2 & \tilde{\gamma}_3 & \tilde{\gamma}_4 & \tilde{\gamma}_5\end{pmatrix} = \begin{pmatrix}\frac{25}{216} & 0 & \frac{1408}{2565} & \frac{2197}{4104} & \frac{-1}{5}\end{pmatrix}$$

while

$$
\begin{aligned}
k_1 &= hf(x_n, y_n),\\
k_2 &= hf(x_n + \tfrac{1}{4}h, y_n + \tfrac{1}{4}k_1),\\
k_3 &= hf(x_n + \tfrac{3}{8}h, y_n + \tfrac{3}{32}k_1 + \tfrac{9}{32}k_2),\\
k_4 &= hf(x_n + \tfrac{12}{13}, y_n + \tfrac{1932}{2197}k_1 - \tfrac{7200}{2197}k_2 + \tfrac{7296}{2197}k_3),\\
k_5 &= hf(x_n + h, y_n + \tfrac{439}{216}k_1 - 8k_2 + \tfrac{3680}{513}k_3 - \tfrac{845}{4104}k_4)
\end{aligned}
$$

and

$$k_6 = hf(x_n + \tfrac{h}{2}, y_n - \tfrac{8}{27}k_1 + 2k_2 - \tfrac{3544}{2565}k_3 + \tfrac{1859}{4104}k_4 - \tfrac{11}{40}k_5).$$

An estimate of the error $\varepsilon_{n+1} = y(x_{n+1}) - y_{n+1}$ can be computed in the following way:

$$\varepsilon_{n+1} \approx y_{n+1} - \tilde{y}_{n+1} = \tfrac{1}{360}k_1 - \tfrac{128}{4275}k_3 - \tfrac{2197}{75240}k_4 + \tfrac{1}{50}k_5 + \tfrac{2}{55}k_6.$$

Runge-Kutta-Fehlberg is a fifth order method.

2.4.5 Reverse Euler

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

assume that f is so simple that y_{n+1} can be isolated in the expression

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1}).$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n, $n = 0, 1, 2, \ldots$, recursively by isolating y_{n+1} in the expression above. Reverse Euler is only a first order method, but has the advantage that it can be used on stiff ODE's.

2.5 Multistep methods for numerical solution of first order ODE's

In numerical multistep methods for solution of first order ODE's, one finds sequences x_n and y_n, with $x_n < x_{n+1}$ such that $y(x_n) \approx y_n$, where y_n is found using $x_{n-1}, \ldots, x_{n-m}$ and $y_{n-1}, \ldots, y_{n-m}$, $m \geq 2$.

2.5.1 Adams-Bashforth methods

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Assume that we know y_1, y_2, and y_3. Define y_n, $n = 4, 5, 6, \ldots$, recursively by

$$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}),$$

where $f_i = f(x_i, y_i)$ for all $i = 0, 1, 2, \ldots$. This is a Adams-Bashforth method of fourth order.

2.5.2 Adams-Moulton methods

Consider the initial value problem

$$y'(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Assume that we know y_1, y_2, and y_3. Define y_n, $n = 4, 5, 6, \ldots$, recursively by

$$\tilde{y}_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$$

and

$$y_{n+1} = y_n + \frac{h}{24}(9\tilde{f}_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}), \tag{19}$$

where $f_i = f(x_i, y_i)$ and $\tilde{f}_i(x_i, \tilde{y}_i)$ for all $i = 0, 1, 2, \ldots$. We can estimate the error in the $(n+1)$'st step $\varepsilon_{n+1} = y(x_{n+1}) - y_{n+1}$ by

$$\varepsilon_{n+1} \approx \frac{1}{15}(y_{n+1} - \tilde{y}_{n+1}).$$

If the error is estimated to be unacceptably large, one can repeat the process by replacing $\tilde{y}_{n+1}$ with y_{n+1}. I.e.

$$\bar{y}_{n+1} = y_n + \frac{h}{24}(9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2})$$

and the new error $\bar{\varepsilon}_{n+1} = y(x_{n+1}) - \bar{y}_{n+1}$ can be estimated by

$$\bar{\varepsilon}_{n+1} \approx \frac{1}{15}(\bar{y}_{n+1} - y_{n+1}).$$

This process can naturally be repeated until one estimates the error to be sufficiently small. This predictor-corrector method is called the Adams-Moulton method of fourth order. The Adams-Moulton method is generally much more precise than an Adams-Bashforth method of same order and is in addition numerically stable.

2.6 Methods for first order systems

In numerical methods for solution of systems of ODE's, one finds sequences x_n and Y_n, where $x_n < x_{n+1}$, such that $Y(x_n) \approx Y_n$.

2.6.1 The Euler-method

Consider the initial value problem

$$Y'(x) = F(x, Y(x)), \qquad \text{where} \qquad Y(x_0) = Y_0,$$

where Y is an unknown d-dimensional vector function, F is a known d-dimensional function of $d+1$ variables, Y_0 is a known d-dimensional vector and x_0 is a known point. Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define Y_n, $n = 0, 1, 2, \ldots$, recursively by

$$Y_{n+1} = Y_n + hF(x_n, Y_n).$$

then the local truncation error is $O(h^2)$ and the global truncation error is $O(h)$. The Euler method is thus a first order method.

2.6.2 RK4

Consider the initial value problem

$$Y'(x) = F(x, Y(x)), \qquad \text{where} \qquad Y(x_0) = Y_0,$$

where Y is an unknown d-dimensional vector function, F is a known d-dimensional function of $d+1$ variables, Y_0 is a known d-dimensional vector and x_0 is a known point. Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define Y_n, $n = 0, 1, 2, \ldots$, recursively by

$$Y_{n+1} = Y_n + \tfrac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4),$$

where

$$\begin{aligned} K_1 &= hF(x_n, Y_n), \\ K_2 &= hF(x_n + \tfrac{1}{2}h, Y_n + \tfrac{1}{2}K_1), \\ K_3 &= hF(x_n + \tfrac{1}{2}h, Y_n + \tfrac{1}{2}K_2) \end{aligned}$$

and

$$K_4 = hF(x_n + h, Y_n + k_3).$$

The RK4 method is a fourth order method with local truncation error $O(h^5)$ and global truncation error $O(h^4)$.

2.6.3 Reverse Euler

Consider the initial value problem

$$Y'(x) = F(x, Y(x)), \qquad \text{where} \qquad Y(x_0) = Y_0.$$

Assume that F is so simple that Y_{n+1} can be isolated in the expression

$$Y_{n+1} = Y_n + hF(x_{n+1}, Y_{n+1}).$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define Y_n, $n = 0, 1, 2, \ldots$, recursively by isolating Y_{n+1} in the expression above. Reverse Euler is only a first order method, but has the advantage that it can be used on stiff ODE's.

2.7 Methods for numerical solution of second order ODE's

In numerical methods to solution of ODE's of second order, one finds sequences x_n, y_n, and y'_n, where $x_n < x_{n+1}$, such that $y(x_n) \approx y_n$ and $y'(x_n) \approx y'_n$.

2.7.1 Runge-Kutta-Nyström methods

2.7.1.1 $y''(x) = f(x, y(x), y'(x))$

Consider the initial value problem

$$y''(x) = f(x, y(x), y'(x)), \qquad \text{where} \qquad y(x_0) = y_0 \quad \text{and} \quad y'(x_0) = y'_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n and y'_n for $n = 0, 1, 2, \ldots$, recursively by

$$y_{n+1} = y_n + h(y'_n + \tfrac{1}{3}(k_1 + k_2 + k_3))$$

and

$$y'_{n+1} = y'_n + \tfrac{1}{3}(k_1 + 2k_2 + 2k_3 + k_4),$$

where

$$\begin{aligned} k_1 &= \tfrac{1}{2}hf(x_n, y_n, y'_n), & k &= \tfrac{1}{2}h(y'_n + \tfrac{1}{2}k_1), \\ k_2 &= \tfrac{1}{2}hf(x_n + \tfrac{1}{2}h, y_n + k, y'_n + k_1), & & \\ k_3 &= \tfrac{1}{2}hf(x_n + \tfrac{1}{2}h, y_n + k, y'_n + k_2), & l &= h(y'_n + k_3) \end{aligned}$$

and

$$k_4 = \tfrac{1}{2}hf(x_n + h, y_n + l, y'_n + 2k_3).$$

This method is called a Runge-Kutta-Nyström method.

2.7.1.2 $y''(x) = f(x, y(x))$

Consider the initial value problem

$$y''(x) = f(x, y(x)), \qquad \text{where} \qquad y(x_0) = y_0 \quad \text{and} \quad y'(x_0) = y'_0.$$

Let $h > 0$ be a step length and put $x_n = x_0 + nh$ for $n = 0, 1, 2, \ldots$. Define y_n and y'_n for $n = 0, 1, 2, \ldots$, recursively by

$$\begin{aligned} k_1 &= \tfrac{1}{2}hf(x_n, y_n), \\ k_2 &= \tfrac{1}{2}hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}h(y'_n + \tfrac{1}{2}k_1)) = k_3, \\ k_4 &= \tfrac{1}{2}hf(x_n + h, y_n + h(y'_n + k_2)), \\ y_{n+1} &= y_n + h(y'_n + \tfrac{1}{3}(k_1 + 2k_2)) \end{aligned}$$

and

$$y'_{n+1} = y'_n + \tfrac{1}{3}(k_1 + 4k_2 + k_4).$$

This method is called a Runge-Kutta-Nyström method.

2.8 Numerical method for the Laplace and Poisson equations in two dimensions

Let $h > 0$ be a step length and let $x_i = x_0 + ih$ and $y_j = y_0 + jh$ for all $i, j \in \mathbb{Z}$, where x_0 and y_0 are possibly 0. The the set of points of the form (x_i, y_j) forms a grid. Assume that the two-dimensional Laplace equation

$$\nabla^2 u = u_{xx} + u_{yy} = 0$$

or the two-dimensional Poisson equation

$$\nabla^2 u = u_{xx} + u_{yy} = f(x, y),$$

has the solution $u(x, y)$ for $(x, y) \in D$, where D is a sufficiently nice subset of $\mathbb{R}^2$. If we for those (i, j) where $(x_i, y_j) \in D$ can find $u_{i,j}$ such that $u(x_i, y_j) \approx u_{i,j}$, then we call the set of these $u_{i,j}$'er a numerical solution to the Laplace- or Poisson equation.

2.8.1 Regular boundary

Denote the boundary of D by ∂D. Assume that we for a suitable choice of x_0, y_0, and $h > 0$ have that every point $(x_i, y_j) \in D$ is either boundary point, $(x_i, y_j) \in \partial D$, or that the four neighbouring points, (x_{i-1}, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), and (x_i, y_{j-1}), also lie in D, and that h is small. Then we can find a numerical solution to the Laplace equation which satisfies the following system of linear equations:

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = 0, \quad \text{for} \quad (i,j) \text{ then } (x_i, y_j) \in D \setminus \partial D, \tag{20}$$

while correspondingly for the Poisson equation, there exists a numerical solution which satisfies the following system of linear equations:

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = h^2 f(x_i,y_j), \quad \text{for} \quad (i,j) \text{ then } (x_i, y_j) \in D \setminus \partial D. \tag{21}$$

Note that (20) corresponds to (21) with $f \equiv 0$.

2.8.1.1 Dirichlet boundary conditions

If we have Dirichlet boundary conditions, i.e. if the values of u are given on the boundary, then we just need to put

$$u_{i,j} = u(x_i, y_j) \quad \text{for} \quad (i,j) \text{ then } (x_i, y_j) \in \partial D, \tag{22}$$

and then solve the system of equations consisting of the equations (20) or (21), and (22).

2.8.1.2 Neumann and mixed boundary conditions

Assume now that we have Neumann boundary conditions on (parts of) the boundary, i.e. we know

$$\frac{\partial u}{\partial n}(x_i, y_j) = n_1 \frac{\partial u}{\partial x} + n_2 \frac{\partial u}{\partial y}$$

instead of $u(x_i, y_j)$ for some (i, j) with $(x_i, y_j) \in \partial D$, where $n = \left(\begin{smallmatrix} n_1 \\ n_2 \end{smallmatrix}\right)$ is a outer normal vector to D. In those points (x_i, y_j) where we have Neumann boundary conditions, (22) is then replaced by

$$\frac{\partial u}{\partial n}(x_i, y_j) = n_1 \frac{u_{i+1,j} - u_{i-1,j}}{2h} + n_2 \frac{u_{i,j+1} - u_{i,j-1}}{2h} \tag{23}$$

and, if it is a Laplace equation,

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = 0, \tag{24}$$

or

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = h^2 f(x_i, y_j), \tag{25}$$

if it is a Poisson equation. Note that some of these values correspond to points outside of D. If D is sufficiently nice, (23) and (24) or (25), where there are Neumann boundary conditions in the point (x_i, y_j), and (22), where there are Dirichlet boundary conditions in the point (x_i, y_j), together with (20) or (21), where $(x_i, y_j) \in D \setminus \partial D$, will give a system of equations with a unique solution.

2.8.2 Irregular boundary

If it doesn't hold that every point $(x_i, y_j) \in D$ is either et boundary point, $(x_i, y_j) \in \partial D$, or that the four neighbouring points, (x_{i-1}, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), and (x_i, y_{j-1}), also lie in D, then the methods obove must be modified.

2.8.2.1 Dirichlet boundary conditions

Assume that $(x_i, y_j) \in D$ is not a boundary point, and that on or more of the neighbouring points (x_{i-1}, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), and (x_i, y_{j-1}) lie outside D.

- If (x_{i+1}, y_j) lies i D, we put $a = 1$, $x_A = x_{i+1}$ and put $u_A = u_{i+1,j}$. Otherwise we choose a, $0 < a < 1$, such that $(x_A, y_j) \in \partial D$, where $x_A = x_i + ah$, and we put $u_A = u(x_A, y_j)$.
- If (x_i, y_{j+1}) lies in D, we let $b = 1$, $y_B = y_{j+1}$ and put $u_B = u_{i,j+1}$. Otherwise we choose b, $0 < b < 1$, such that $(x_i, y_B) \in \partial D$, where $y_B = y_j + bh$, and we put $u_B = (x_i, y_B)$.
- If (x_{i-1}, y_j) lies in D, we let $p = 1$, $x_P = x_{i-1}$ and put $u_P = u_{i-1,j}$. Otherwise we choose p, $0 < p < 1$, such that $(x_P, y_j) \in \partial D$, where $x_P = x_i - ph$, and we put $u_P = u(x_P, y_j)$.
- If (x_i, y_{j-1}) lies in D, we let $q = 1$, $y_Q = y_{j-1}$ and put $u_Q = u_{i,j-1}$. Otherwise we choose q, $0 < q < 1$, such that $(x_i, y_Q) \in \partial D$, where $y_Q = y_j - qh$, and we put $u_Q = u(x_i, y_Q)$.

We can then find a numerical solution which satisfies the following equation:

$$\frac{u_A}{a(a+p)} + \frac{u_B}{b(b+q)} + \frac{u_P}{p(p+a)} + \frac{u_Q}{q(q+b)} - \frac{ap+bq}{abpq} u_{i,j} = 0, \tag{26}$$

if it is the Laplace equation, and

$$\frac{u_A}{a(a+p)} + \frac{u_B}{b(b+q)} + \frac{u_P}{p(p+a)} + \frac{u_Q}{q(q+b)} - \frac{ap+bq}{abpq} u_{i,j} = \frac{h^2}{2} f(x_i, y_j), \tag{27}$$

if it is a Poisson equation. For all (i, j), where (x_i, y_j) is not a boundary point, and one or more of the neighbouring points (x_{i-1}, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), and (x_i, y_{j-1}) lie outside of D, we now use either the equation (26) or (27), and for alle (i, j), where (x_i, y_j) is not a boundary point, and (x_{i-1}, y_j), (x_{i+1}, y_j), (x_i, y_{j-1}), and (x_i, y_{j-1}) lie inside of D, we use the equation (20) or (21). Together with (22) we then get a system of linear equations with a unique solution.

2.8.3 The Gauss-Seidel iterationsmethod

We need to solve a system of linear equations to find the solutions above, possibly with many (N) equations and many (N) unknowns. Write the system of linear equations on the form $Ax = b$, where $A = (a_{i,j})_{i,j=1}^{N}$ is an $N \times N$-matrix, x is a vector consisting of the unknown values, and $b = \begin{pmatrix} b_1 & b_2 & \dots & b_N \end{pmatrix}$ is a known vector. The Gauss-Seidel iterationsmethod finds a numerical solution to the system of equations $Ax = b$ by means of of the following iterative method.

1. first one makes a guess for a solution, which is called $x^{(0)}$ and n is put to 0.
2. One then finds $x^{(n)} = \begin{pmatrix} x_1^{(n+1)} & x_2^{(n+1)} & \dots & x_N^{(n+1)} \end{pmatrix}$ in the following way:
   - First put $x_1^{(n+1)} = \frac{1}{a_{1,1}}(b_1 - \sum_{j=2}^{N} a_{1,j} x_j^{(n)})$.

- Second $x_2^{(n+1)} = \frac{1}{a_{2,2}}(b_2 - \sum_{j=1}^{1} a_{2,j}x_j^{(n+1)} - \sum_{j=3}^{N} a_{2,j}x_j^{(n)})$.
- and so on: $x_i^{(n+1)} = \frac{1}{a_{i,i}}(b_i - \sum_{j=1}^{i-1} a_{i,j}x_j^{(n+1)} - \sum_{j=i+1}^{N} a_{i,j}x_j^{(n)})$ for $i = 3, \ldots, N-1$.
- and lastly $x_N^{(n+1)} = \frac{1}{a_{N,N}}(b_N - \sum_{j=1}^{N-1} a_{N,j}x_j^{(n+1)})$.

3. Now replace n with $n+1$ and repeat the process from step 2.

In many cases (e.g. if A is so-called *symmetric positive-definite* or *diagonally dominant*), then the sequence $x^{(n)}$ will tend to the unique solution for the system of equations $Ax = b$. In pratice, one stops the process when $x^{(n+1)}$ is almost equal to $x^{(n)}$.