Lecture Notes in TMA4215
Numerical Mathematics

November 25, 2011

Abstract

These lecture notes are supplementary to the text book used in the course Numerical Mathematics. The notes focus on numerical solution of ordinary differential equations.The original version of these notes was written in Norwegian by Brynjulf Owren. The material has been substantially amended by Anne Kværnø and lately also by Elena Celledoni.

Contents

1 Eulers method. 3

2 Some background on ODEs. 7

3 Numerical solution of ODEs. 8
3.1 Some examples of one-step methods. 9

4 Runge-Kutta methods 10
4.1 Order conditions for Runge-Kutta methods. 12
4.2 Error control and stepsize selection. 15

5 Stiff equations and linear stability 18

6 Linear multistep methods 23
6.1 Consistency and order. 24
6.2 Linear difference equations 25
6.3 Zero-stability and convergence 27
6.4 Adams-Bashforth-Moulton methods 28
6.5 Predictor-corrector methods 29

7 Orthogonal polynomials. 31

8 Solution of systems of nonlinear equations 34

9 Bernoulli polynomials and the Euler-Maclaurin formula. 38

10 Linear algebra: introduction 40

11 Stability of linear systems 41
11.1 Preliminaries 41
11.2 Stability analysis 42

12 Gaussian elimination 44
12.1 Example 45
12.2 Gauss elimination: general algorithm 47
12.3 Gaussian elimination with partial pivoting 48
12.4 Two exmples: Gaussian elimination with partial pivoting 48
12.5 G-E with partial pivoting: general algorithm 50
12.6 Complexity of Gaussian elimination 51

13 Other matrix factorizations 52

14 Symmetric matrices 53
14.1 Positive definite matrices 53

15 Gershgorin's theorem 54

16 Solution of linear systems by iteration **55**
16.1 Example 55
16.2 Example 56
16.3 Convergence 57
16.4 Example 57
16.5 Example 57

17 Krylov subspace methods **59**

18 Preconditioning **59**

1 Eulers method.

Let us start this introduction to the numerical solution of *ordinary differential equations* (ODEs) by something familiar. Given a scalar (one equation only) ODE

$$y' = f(t, y), \qquad t_0 \le t \le t_{end}, \qquad y(t_0) = y_0, \tag{1}$$

in which the function f, the integration interval $[t_0,t_{end}]$ and the initial value y_0 is assumed to be given. The *solution* of this initial value problem (IVP) is a function $y(t)$ on the interval $[t_0, t_{end}]$.

Example 1.1. *The ODE/IVP*

$$y' = -2ty, \qquad 0 \le t \le 1, \qquad y(0) = 1.0$$

has as solution the function

$$y(t) = e^{-t^2}.$$

But in many practical situations, it is not possible to express the solution $y(t)$ in closed form, even if a solution exist. In these cases, a numerical algorithm can give an *approximation* to the exact solution. Let us start with Eulers method, which should be known from some calculus classes. Divide the interval $[t_0, t_{end}]$ into $Nstep$ equal subintervals, each of size $h = (t_{end} - t_0)/Nstep$, and let $t_n = t_0 + nh$. Euler's method can be derived by several means. One possibility is to use the first few terms of the Taylor expansion of the exact solution, which is given by

$$y(t_0+h) = y(t_0)+hy'(t_0)+\frac{1}{2}h^2y''(t_0)+\cdots+\frac{1}{p!}h^py^{(p)}(t_0)+\frac{1}{(p+1)!}h^{p+1}y^{(p+1)}(\xi), \tag{2}$$

where ξ is somewhere between t_0 and t_{end}. The integer $p \ge 1$ is a number of our own choice, but we have to require y to be sufficiently differentiable, in this case that $y^{(p+1)}$ exist and is continuous. If h is small, we may assume that the solution will be completely dominated by the first two terms, thus

$$y(t_0 + h) \approx y(t_0) + hy'(t_0) = y_0 + hf(t_0, y_0),$$

and we call this approximate solution y_1. Starting from the point $t_1 = t_0+h$ and y_1 we can repeat the process. We have now developed Euler's method, given by

$$y_{n+1} = y_n + hf(t_n, y_n), \qquad n = 0, 1, \cdots, Nsteps - 1,$$

resulting in approximations $y_n \approx y(t_n)$.

Example 1.2. *Eulers method with* $h = 0.1$ *applied to the ODE of Example 1.1 gives*

t_n	y_n
0.0	1.0000
0.1	1.0000
0.2	0.9800
0.3	0.9408
0.4	0.8844
0.5	0.8136
0.6	0.7322
0.7	0.6444
0.8	0.5542
0.9	0.4655
1.0	0.3817

.

In this case we know the exact solution, $y(1.0) = e^{-1.0^2} = 0.3679$ *and the error at the endpoint is* $e_{10} = y(1.0) - y_{10} = -1.38 \cdot 10^{-2}$*. If we repeat this experiment (write a MATLAB program to do so) with different stepsizes, and measure the error at the end of the interval, we get*

h	$e_{Nstep} = y(1.0) - y_{Nstep}$
0.1	$-1.38 \cdot 10^{-2}$
0.05	$-6.50 \cdot 10^{-3}$
0.025	$-3.16 \cdot 10^{-3}$
0.0125	$-1.56 \cdot 10^{-3}$

.

From this example, it might look like the error at the endpoint $e_{Nstep} \sim h$, where $h = (tend - t_0)/Nstep$. But is this true for all problems, and if yes, can we prove it? To do so, we need to see what kind of errors we have and how they behave. This is illustrated in Figure 1. For each step an error is made, and these errors are then propagated til the next steps and accumulate at the endpoint.

Definition 1.3. *The* local truncation error d_{n+1} *is the error done in one step when starting at the exact solution* $y(t_n)$*. The* global error *is the difference between the exact and the numerical solution at point* t_n*, thus* $e_n = y(t_n) - y_n$*.*

The local truncation error of Euler's method is

$$d_{n+1} = y(t_n + h) - y(t_n) - hf(t_n, y(t_n)) = \frac{1}{2}h^2 y''(\xi),$$

where $\xi \in (t_n, t_{n+1})$. This is given from the Taylor-expansion of $y(t_n+h)$ around t_n with $p = 1$. To see how the global error propagates from one step to the next, the trick is: We have

$$\begin{aligned} y(t_n + h) &= y(t_n) + hf(t_n, y(t_n)) + d_{n+1}, \\ y_{n+1} &= y_n + hf\left(t_n, y_n\right). \end{aligned}$$

Take the difference of these two, and get

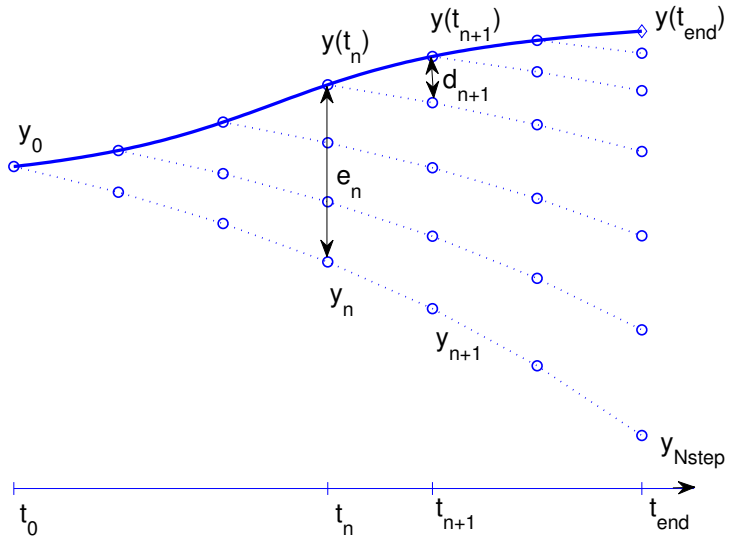


Figure 1: Lady Windermere's Fan

$$e_{n+1} = e_n + h\left(f\left(t_n, y(t_n)\right) - f\left(t_n, y_n\right)\right) + d_{n+1} = (1 + hf_y(t_n, v))e_n + d_{n+1}, \quad (3)$$

where v is somewhere between $y(t_n)$ and y_n. We have here used the mean value theorem (Theorem 1.8 in Burden and Faires) for $f\left(t_n, y(t_n)\right) - f\left(t_n, y_n\right)$. This is about as far as we get with exact calculations, since ξ in d_{n+1} as well as v in f_y are unknown, and will also change from one step to the next. So we will look for an *upper bound* of the global error. We will first assume upper bounds for our unknown, that is, we assume there exist positive constants D and L so that

$$\frac{1}{2}\left|y''\right| \leq D \text{ for all } t \in (t_0, t_{end}) \qquad \text{and} \qquad |f_y| \leq L \text{ for all } t \in [t_0, t_{end}] \text{ and for all } y.$$

Taken the absolute value of both sides of (3) and using the triangle inequality gives

$$|e_{n+1}| \leq (1 + hL)\,|e_n| + Dh^2.$$

Since $e_0 = 0$ (there is no error at the initial point) we can use this formula recursively to get an upper bound for the error at the endpoint:

$$\begin{aligned}
|e_1| &\leq Dh^2, \\
|e_2| &\leq (1 + hL)Dh^2 + Dh^2 \\
&\vdots \\
|e_{Nstep}| &\leq \sum_{i=0}^{Nstep-1} (1 + hL)^i Dh^2 = \frac{(1 + hL)^{Nstep} - 1}{1 + hL - 1} Dh^2.
\end{aligned}$$

Using the fact that $1 + hL \leq e^{hL}$ (why?) and $h \cdot Nstep = t_{end} - t_0$ we finally reach the conclusion

$$|e_{Nstep}| \leq \frac{\left(e^{hL}\right)^{Nstep} - 1}{L} Dh = \frac{e^{L(t_{end}-t_0)} - 1}{L} D \cdot h = C \cdot h.$$

The constant $C = \left(e^{hL} - 1\right) D/L$ depends only on the problem, and we have proved convergence

$$|y(t_{end}) - y_{Nstep}| \to 0 \text{ when } \ h \to 0 \text{ (or } Nstep \to \infty).$$

Summary: In this section we have

1. Formulated the problem.
2. Developed an algorithm.
3. Implemented and tested it.
4. Proved convergence.

This is fairly much what this course in Numerical Mathematics is about. To be more precise, for each class of problems (ODEs, integrals, linear and nonlinear equations,$\cdots$) we will roughly do the following

1. Formulate the problem. What do we know about it? What about existence and uniqueness results?
2. Develop an algorithm to find a solution. Can it be generalised?
3. Implement and test the algorithm. Test it on problems with known solutions. Do we get a reasonable result?
4. Prove convergence. How accurate is the algorithm?
5. Verify the theoretical results by numerical experiments.
6. Try the algorithm on harder problems. Do we get unexpected results? If yes, can they be explained? Can we get around them?
7. Can we make our algorithm to automatically adjust itself to fulfil requirements given by the user (adaptivity)?

The last two points do not apply to all the problems we are going to discuss. We will also derive mathematical results that are useful for either the theoretical analysis, or for development of methods.

2 Some background on ODEs.

In this section some useful notation on ordinary differential equations will be presented. We will also give existence and uniqueness results, but without proofs.

A system of m first order ordinary differential equation is given by

$$y' = f(t, y) \tag{4}$$

or, written out, as

$$\begin{aligned} y_1' &= f_1(t, y_1, \cdots, y_m), \\ y_2' &= f_2(t, y_1, \cdots, y_m), \\ &\vdots \\ y_m' &= f_m(t, y_1, \cdots, y_m). \end{aligned}$$

This is an *initial value problem* (IVP) if the solution is given at some point t_0, thus

$$y_1(t_0) = y_{1,0},\ y(t_0) = y_{2,0},\ \cdots\ y_m(t_0) = y_{m,0}.$$

Example 2.1. *The following equation is an example of the Lotka-Volterra equation:*

$$\begin{aligned} y_1' &= y_1 - y_1 y_2, \\ y_2' &= y_1 y_2 - 2y_2. \end{aligned}$$

An ODE is called *autonomous* if f is not a function of t, but only of y. The Lotka-Volterra equation is an example of an autonomous ODE. A nonautonomous system can be made autonomous by a simple trick, just add the equation

$$y_{m+1}' = 1, \qquad y_{m+1}(t_0) = t_0,$$

and replace t with y_{m+1}. Also higher order ODE/IVPs

$$u^{(m)} = f(t, u, u', \cdots, u^{(m-1)}), \qquad u(t_0) = u_0,\ u'(t_0) = u_0',\ \cdots, u^{(m-1)}(t_0) = u_0^{(m-1)},$$

where $u^{(m)} = d^m u/dt^m$, can be written as a system of first order equations, again by a simple trick: Let

$$y_1 = u,\ y_2 = u',\ \cdots y_m = u^{(m-1)},$$

and we get the system

$$\begin{aligned} y_1' &= y_2, & y_1(t_0) &= u_0, \\ y_2' &= y_3, & y_2(t_0) &= u_0', \\ &\vdots & &\vdots \\ y_{m-1}' &= y_m, & y_{m-1}(t_0) &= u_0^{(m-2)}, \\ y_m' &= f(t, y_1, y_2, \cdots, y_m), & y_m(t_0) &= u_0^{(m-1)}. \end{aligned}$$

Example 2.2. *Van der Pol's equation is given by*

$$u'' + \mu(u^2 - 1)u' + u = 0.$$

Using $y_1 = u$ *and* $y_2 = u'$ *this equation can be rewritten as*

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= \mu(1 - y_1^2)y_2 - y_1. \end{aligned}$$

This problem was first introduced by Van der Pol in 1926 in the study of an electronic oscillator.

Before concluding this section, we present some existence and uniqueness results for solution of ODEs.

Definition 2.3. *A function* $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ *satisfies the* Lipschitz condition *with respect to* y *on a domain* $(a, b) \times D$ *where* $D \subset \mathbb{R}^m$ *if there exist a constant* L *so that*

$$\|f(t, y) - f(t, \tilde{y})\| \leq L\|y - \tilde{y}\|, \qquad \text{for all} \quad t \in (a, b),\ y, \tilde{y} \in D.$$

The constant L *is called* the Lipschitz constant.

It is not hard to show that the function f satisfies the Lipschitz condition if $\partial f_i/\partial y_j,\ i, j = 1, \cdots, m$ are continuous and bounded on the domain.

Theorem 2.4. *Consider the initial value problem*

$$y' = f(t, y), \qquad y(t_0) = y_0. \tag{5}$$

If

1. $f(t, y)$ *is continuous in* $(a, b) \times D$,
2. $f(t, y)$ *satisfies the Lipschitz condition with respect to* y *in* $(a, b) \times D$.

with given initial values $t_0 \in (a, b)$ *and* $y_0 \in D$, *then* (5) *has one and only one solution in* $(a, b) \times D$.

3 Numerical solution of ODEs.

In this section we develop some simple methods for the solution of initial value problems. In both cases, let us assume that we somehow have found solutions $y_l \approx y(t_l)$, for $l = 0, 1, \cdots, n$, and we want to find an approximation $y_{n+1} \approx y(t_{n+1})$ where $t_{n+1} = t_n + h$, where h is the stepsize. Basically, there are two different classes of methods in practical use.

1. *One-step methods.* Only y_n is used to find the approximation y_{n+1}. One-step methods usually require more than one function evaluation pr. step. They can all be put in a general abstract form

$$y_{n+1} = y_n + h\Phi(t_n, y_n; h).$$

2. *Linear multistep methods:* y_{n+1} is approximated from $y_{n-k+1}, \cdots, y_n$.

3.1 Some examples of one-step methods.

Assume that t_n, y_n is known. The exact solution $y(t_{n+1})$ with $t_{n+1} = t_n + h$ of (4) passing through this point is given by

$$y(t_n + h) = y_n + \int_{t_n}^{t_{n+1}} y'(\tau)d\tau = y_n + \int_{t_n}^{t_{n+1}} f(\tau, y(\tau))d\tau. \tag{6}$$

The idea is to find approximations to the last integral. The simplest idea is to use $f(\tau, y(\tau)) \approx f(t_n, y_n)$, in which case we get the Euler method again:

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

The integral can also be approximated by the trapezoidal rule

$$\int_{t_n}^{t_{n+1}} f(\tau, y(\tau)) = \frac{h}{2}(f(t_n, y_n) + f(t_{n+1}, y(t_{n+1})).$$

By replacing the unknown solution $y(t_{n+1})$ by y_{n+1} we get the *trapezoidal method*

$$y_{n+1} = y_n + \frac{h}{2}\left(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right).$$

Here y_{n+1} is available by solving a (usually) nonlinear system of equations. Such methods are called implicit. To avoid this extra difficulty, we could replace y_{n+1} on the right hand side by the approximation from Eulers method, thus

$$\begin{aligned}\tilde{y}_{n+1} &= y_n + hf(t_n, y_n);\\ y_{n+1} &= y_n + \frac{h}{2}\left(f(t_n, y_n) + f(t_{n+1}, \tilde{y}_{n+1})\right).\end{aligned}$$

This method is called the *improved Euler method*. Similarly, we could have used the midpoint rule for the integral,

$$\int_{t_n}^{t_{n+1}} f(\tau, y(\tau)) = \left(f(t_n + \frac{h}{2}, y(t_n + \frac{h}{2})\right),$$

and replaced $y(t_n + \frac{h}{2})$ by one half Euler step. The result is the *modified Euler method*:

$$\begin{aligned}\tilde{y}_{n+\frac{1}{2}} &= y_n + \frac{h}{2}f(t_n, y_n),\\ y_{n+1} &= y_n + hf(t_n + \frac{h}{2}, \tilde{y}_{n+\frac{1}{2}}).\end{aligned}$$

Do we gain anything by constructing these methods? Let us solve the problem from Example 1.1 using improved/modified Euler with $h = 0.1$. For each step, also the global error $e_n = y(t_n) - y_n$ is computed. For comparison, also the

result for the Euler method is included.

	Euler		improved Euler		modified Euler	
t_n	y_n	e_n	y_n	e_n	y_n	e_n
0.0	1.000000	0	1.000000	0	1.000000	0
0.1	1.000000	$-9.95 \cdot 10^{-3}$	0.990000	$4.98 \cdot 10^{-5}$	0.990000	$4.98 \cdot 10^{-5}$
0.2	0.980000	$-1.92 \cdot 10^{-2}$	0.960696	$9.34 \cdot 10^{-5}$	0.960597	$1.92 \cdot 10^{-4}$
0.3	0.940800	$-2.69 \cdot 10^{-2}$	0.913814	$1.17 \cdot 10^{-4}$	0.913528	$4.03 \cdot 10^{-4}$
0.4	0.884352	$-3.22 \cdot 10^{-2}$	0.852040	$1.04 \cdot 10^{-4}$	0.851499	$6.45 \cdot 10^{-4}$
0.5	0.813604	$-3.48 \cdot 10^{-2}$	0.778765	$3.60 \cdot 10^{-5}$	0.777930	$8.71 \cdot 10^{-4}$
0.6	0.732243	$-3.46 \cdot 10^{-2}$	0.697773	$-9.69 \cdot 10^{-5}$	0.696636	$1.04 \cdot 10^{-3}$
0.7	0.644374	$-3.17 \cdot 10^{-2}$	0.612924	$-2.98 \cdot 10^{-4}$	0.611507	$1.12 \cdot 10^{-3}$
0.8	0.554162	$-2.69 \cdot 10^{-2}$	0.527850	$-5.58 \cdot 10^{-4}$	0.526202	$1.09 \cdot 10^{-3}$
0.9	0.465496	$-2.06 \cdot 10^{-2}$	0.445717	$-8.59 \cdot 10^{-4}$	0.443904	$9.54 \cdot 10^{-4}$
1.0	0.381707	$-1.38 \cdot 10^{-2}$	0.369053	$-1.17 \cdot 10^{-3}$	0.367153	$7.27 \cdot 10^{-4}$

As we can see, there is a significant improvement in accuracy, compared with the Euler method.

4 Runge-Kutta methods

The Euler method, as well as the improved and modified Euler methods are all examples on *explicit Runge-Kutta methods* (ERK). Such schemes are given by

$$\begin{aligned} k_1 &= f(t_n, y_n), \\ k_2 &= f(t_n + c_2 h, y_n + h a_{21} k_1), \\ k_3 &= f\big(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)\big), \\ &\vdots \\ k_s &= f\big(t_n + c_s h, y_n + h \sum_{j=1}^{s-1} a_{sj} k_j\big), \\ y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i k_i, \end{aligned} \tag{7}$$

where c_i, a_{ij} and b_i are coefficients defining the method. We always require $c_i = \sum_{j=1}^{s} a_{ij}$. Here, s is the number of *stages*, or the number of function evaluations needed for each step. The vectors k_i are called stage derivatives. The improved Euler method is then a two-stage RK-method, written as

$$\begin{aligned} k_1 &= f(t_n, y_n), \\ k_2 &= f(t_n + h, y_n + h k_1), \\ y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2). \end{aligned}$$

Also implicit methods, like the trapezoidal rule,

$$y_{n+1} = y_n + \frac{h}{2}\big(f(t_n, y_n) + f(t_n + h, y_{n+1})\big)$$

can be written in a similar form,

$$\begin{aligned} k_1 &= f(t_n, y_n), \\ k_2 &= f\big(t_n + h, y_n + \frac{h}{2}(k_1 + k_2)\big), \\ y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2). \end{aligned}$$

But, contrary to what is the case for explicit methods, a nonlinear system of equations has to be solved to find k_2.

Definition 4.1. *An s-stage Runge-Kutta method is given by*

$$k_i = f\big(t_n + c_i h, y_n + h\sum_{j=1}^{s} a_{ij}k_j\big), \qquad i = 1, 2, \cdots, s,$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i.$$

The method is defined by its coefficients, which is given in a Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}, \qquad \text{where } c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1, \cdots, s.$$

The method is explicit *if $a_{ij} = 0$ whenever $j \geq i$, otherwise* implicit.

Example 4.2. *The Butcher-tableaux for the methods presented so far are*

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Euler *improved Euler* *modified Euler* *trapezoidal rule*

When the method is explicit, the zeros on and above the diagonal is usually ignored. We conclude this section by presenting the maybe most popular among the RK-methods over times, *The* 4th order Runge-Kutta method (Kutta – 1901):

$$\begin{aligned} k_1 &= f(t_n, y_n) \\ k_2 &= f(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}k_1) \\ k_3 &= f(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}k_2) \\ k_4 &= f(t_n + h, y_n + hk_3) \\ y_{n+1} &= y_n + \tfrac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{aligned} \qquad \text{or} \qquad \begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} . \tag{8}$$

4.1 Order conditions for Runge-Kutta methods.

The following theorem were proved in Exercise 2, task 2:

Theorem 4.3. *Let*

$$y' = f(t, y), \qquad y(t_0) = y_0, \qquad t_0 \le t \le t_{end}$$

be solved by a one-step method

$$y_{n+1} = y_n + h\Phi(t_n, y_n; h), \tag{9}$$

with stepsize $h = (t_{end} - t_0)/Nstep$. *If*

1. *the increment function* Φ *is Lipschitz in* y, *and*
2. *the local truncation error* $d_{n+1} = \mathcal{O}(h^{p+1})$,

then the method is of order p, *that is, the global error at* t_{end} *satisfies*

$$e_{Nstep} = y(t_{end}) - y_{Nstep} = \mathcal{O}(h^p).$$

A RK method is a one-step method with increment function $\Phi(t_n, y_n; h) = \sum_{i=1}^{s} b_i k_i$. It is possible to show that Φ is Lipschitz in y whenever f is Lipschitz and $h \le h_{max}$, where h_{max} is some predefined maximal stepsize. What remains is the order of the local truncation error. To find it, we take the Taylor-expansions of the exact and the numerical solutions and compare. The local truncation error is $\mathcal{O}(h^{p+1})$ if the two series matches for all terms corresponding to h^q with $q \le p$. In principle, this is trivial. In practise, it becomes extremely tedious (give it a try). Fortunately, it is possible to express the two series very elegant by the use of *B-series* and *rooted trees*. Here, we present how this is done, but not why it works. A complete description can be found in the note *the B-series tutorial*.

B-series and rooted trees

We assume that the equation is rewritten in autonomous form

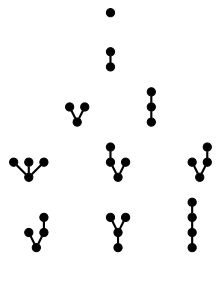
$$y(t)' = f(y(t)), \qquad y(t_0) = y_0. \tag{10}$$

The Taylor expansion of the exact solution of (10) is given by

$$y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{h}{2}y''(t_0) + \cdots + \frac{h^p}{p!}y^{(p)}(t_0) + \cdots . \tag{11}$$

From the ODE (10) and repeated use of the chain rule, we get $y' = f$, $y'' = f_y f$, $y''' = f_{yy}ff + f_y f_y f$, etc. Each higher derivative of y is split into several terms, denoted as *elementary differentials*. These can be represented by rooted trees. A node $\bullet$ represents f. A branch out from a bullet represent the derivative of f with respect to y. As the chain rule apply, this will always mean that we

multiply by $y' = f$, represented by a new node on the end of the branch. We get the following table:

Elementary differentials	corresponding trees
$y' = f$	
$y'' = f_y f$	
$y''' = f_{yy}ff + f_y f_y f$	
$y^{iv} = f_{yyy}fff + f_{yy}f_y ff + f_{yy}ff_y f$	
$+f_{yy}ff_y f + f_y f_{yy} ff + f_y f_y f_y f$	

The elementary differentials corresponding to the trees  and  are equal, thus

$$y^{iv} = f_{yyy}fff + 3f_{yy}f_y ff + f_y f_{yy} ff + f_y f_y f_y f.$$

And we can go on like that. For each tree τ with p nodes we construct a set of total p new trees with $p+1$ nodes by adding one new node to an existing node in τ. This procedure might produce the same tree several times, and the total number of ways to construct a distinct tree is denoted by $\alpha(\tau)$. Let T be the set of all possible, distinct, rooted trees constructed this way, and let $\tau \in T$. A tree with p nodes corresponds to one of the terms in $y^{(p)}$, thus we call this *the order* of the tree and denote it $|\tau|$. The elementary differentials corresponding to a tree is denoted $F(\tau)(y)$.

Example 4.4.

For $\tau =$  *we have* $|\tau| = 4, \qquad F(\tau)(y) = f_y f_{yy} ff, \qquad \alpha(\tau) = 1.$

For $\tau =$  *we have* $|\tau| = 4, \qquad F(\tau)(y) = f_{yy} f_y ff, \qquad \alpha(\tau) = 3.$

Here, f and its differentials are evaluated in y.

Putting this together: If $y(t)$ is the solution of (10), then

$$y^{(p)}(t_n) = \sum_{\substack{\tau \in T \\ |\tau| = p}} \alpha(\tau) F(\tau)(y(t_n)).$$

Insert this into (11), and we can write the exact solution as a B-series:

$$y(t_n + h) = y(t_n) + \sum_{\tau \in T} \frac{h^{|\tau|}}{|\tau|!}\, \alpha(\tau)\, F(\tau)(y(t_n)). \tag{12}$$

The numerical solution after one step can also be written as a B-series, but with some different coefficients

$$y_{n+1} = y_n + \sum_{\tau \in T} \frac{h^{|\tau|}}{|\tau|!}\, \gamma(\tau)\varphi(\tau)\, \alpha(\tau)\, F(\tau)(y_n). \tag{13}$$

where $\gamma(\tau)$ is an integer, and $\varphi(\tau)$ depends on the method coefficients, given in the Butcher tableau in Definition 4.1. Both can be found quite easily by the following procedure: Take a tree τ. Label the root with i, and all other non-terminal nodes by $j, k, l, \cdots$. The root correspond to b_i. A branch between a lower node j and an upper node k correspond to a_{jk}. A terminal node, connected to a node with label k corresponds to c_k. $\phi(\tau)$ is found by multiplying all these coefficients, and then take the sum over all the indices from 1 to s.

Example 4.5.

The tree $\tau =$  *can be labelled so that* $\varphi(\tau) = \sum_{i,j,k,l=1}^{s} b_i a_{ij} a_{jk} a_{il}$.

A tree τ can also be described by its subtrees. Let $\tau = [\tau_1, \tau_2, \cdots, \tau_l]$ be the tree composed by joining the root of the subtrees $\tau_1,\ \tau_2,\ \cdots,\ \tau_l$ to a joint new root. The term $\gamma(\tau)$ is defined recursively by

- $\gamma(\bullet) = 1$.
- $\gamma(\tau) = |\tau| \cdot \gamma(\tau_1) \cdots \gamma(\tau_l)$ for $\tau = [\tau_1, \tau_2, \cdots, \tau_l]$.

Example 4.6.

$\tau =$ $= [\bullet]$, $\qquad \gamma(\tau) = 2 \cdot 1 = 2$

$\tau =$ $= [\bullet, \bullet]$, $\qquad \gamma(\tau) = 3 \cdot 1 \cdot 1 = 3$

$\tau =$ $= [$  $]$ $\qquad \gamma(\tau) = 4 \cdot 3 = 12$

$\tau =$ $= [$$,$$]$, $\qquad \gamma(\tau) = 7 \cdot 12 \cdot 2 = 168$

By comparing the two series (12) and (13) with $y(t_n) = y_n$ we can state the following theorem:

Theorem 4.7. *A Runge-Kutta method is of order p if and only if*

$$\varphi(\tau) = \frac{1}{\gamma(\tau)} \qquad \forall \tau \in T, \quad |\tau| \le p.$$

The order conditions up to order 4 are:

τ	$\lvert\tau\rvert$	$\varphi(\tau) = 1/\gamma(\tau)$
	1	$\sum b_i = 1$
	2	$\sum b_i c_i = 1/2$
	3	$\sum b_i c_i^2 = 1/3$
		$\sum b_i a_{ij} c_j = 1/6$
	4	$\sum b_i c_i^3 = 1/4$
		$\sum b_i c_i a_{ij} c_j = 1/8$
		$\sum b_i a_{ij} c_j^2 = 1/12$
		$\sum b_i a_{ij} a_{jk} c_k = 1/24$

4.2 Error control and stepsize selection.

A user of some numerical black box software will usually require one thing: The accuracy of the numerical solution should be within some user specified tolerance. To accomplish this we have to measure the error, and if the error is too large, it has to be reduced. For ordinary differential equations, this means to reduce the stepsize. On the other hand, we would like our algorithm to be as efficient as possible, that is, to use large stepsizes. This leaves us with two problems: How to measure the error, and how to get the right balance between accuracy and efficiency.

Local error estimate. As demonstrated in Figure 1, the global error $y(t_n) - y_n$ comes from two sources: the local truncation error and the propagation of errors produced in preceding steps. This makes it difficult (but not impossible) to measure the global error. Fortunately it is surprisingly easy to measure the *local error*, l_{n+1}, the error produced in one step when starting at (t_n, y_n), see Figure 2. Let $y(t; t_n, y_n)$ be the exact solution of the ODE through the point t_n, y_n. For a method of order p we get

$$l_{n+1} = y(t_n + h; t_n, y_n) - y_{n+1} = \Psi(t_n, y_n)h^{p+1} + \mathcal{O}(h^{p+2}),$$

where $\mathcal{O}(h^{p+1})$ refer to higher order terms [1] The term $\Psi(t_n, y_n)h^{p+1}$ is called *the principal error term*, and we assume that this term is the dominating part of the error. This assumption is true if the stepsize h is sufficiently small. Taking a step from the same point t_n, y_n with a method of order $\hat{p} = p + 1$ gives a solution $\hat{y}_{n+1}$ with a local error satisfying

$$y(t_n + h; t_n, y_n) - \hat{y}_{n+1} = \mathcal{O}(h^{p+2}).$$

The *local error estimate* is given by

$$le_{n+1} = \hat{y}_{n+1} - y_{n+1} = \Psi(t_n, y_n)h^{p+1} + \mathcal{O}h^{p+2} \approx l_{n+1}.$$

Embedded Runge-Kutta pair Given a Runge-Kutta method of order p. To be able to measure the local error, we need a method of order $p + 1$ (or higher). But we do not want to spend more work (in terms of f-evaluations) than necessary. The solution is *embedded Runge-Kutta pairs*, which, for explicit

[1] Strictly speaking, the Landau-symbol $\mathcal{O}$ is defined by

$$f(x) = \mathcal{O}(g(x)) \quad \text{for } x \to x_0 \qquad \text{if} \qquad \lim_{x \to x_0} \frac{\|f(x)\|}{\|g(x)\|} < K < \infty$$

for some unspecified constant K. Thus $f(h) = \mathcal{O}(h^q)$ means that $\|f(h)\| \leq Kh^q$ when $h \to 0$, and refer to the remainder terms of a truncated series.

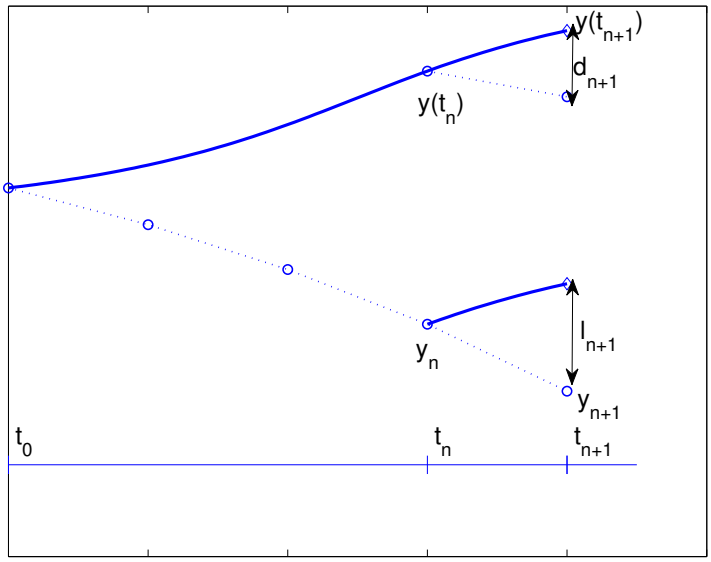


Figure 2: Lady Windermere's Fan

methods are given by

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & & \ddots & & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & \\ \hline & \hat{b}_1 & \hat{b}_2 & \cdots & \hat{b}_{s-1} & \hat{b}_s \end{array}$$

The method given by the b_i's is of order p, the error estimating method given by the $\hat{b}_i$'s is of order $p+1$. (Sometimes it is the other way round. The important thing is to have two methods of different order.) The local error estimate of y_{n+1} is then given by

$$le_{n+1} = \hat{y}_{n+1} - y_{n+1} = h \sum_{i=1}^{s} (\hat{b}_i - b_i) k_i.$$

Example 4.8. *A combination of the Euler method and improved Euler will result in the following pair*

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

so that

$$k_1 = f(t_n, y_n), \quad k_2 = f(t_n+h, y_n+hk_1), \quad y_{n+1} = y_n+hk_1, \quad l_{n+1} \approx le_{n+1} = \frac{h}{2}(-k_1+k_2).$$

Example 4.9. *Assume that you have decided to use improved Euler, which is of order 2, as your advancing method, and you would like to find an error estimating method of order 3. There are no 2-stage order 3 ERKs, so you have to add one stage to your method. This gives a method like*

$$\begin{array}{c|ccc} 0 & & & \\ 1 & 1 & & \\ c_3 & a_{31} & a_{32} & \\ \hline & \frac{1}{2} & \frac{1}{2} & \\ \hline & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 \end{array}$$

where we require $c_3 = a_{31} + a_{32}$, which give us five free parameters. These have to satisfy all four order condition for an order 3 method. Using c_3 as a free parameter, we get the following class of 3rd order methods:

$$b_1 = \frac{3c_3 - 1}{6c_3}, \quad b_2 = \frac{2 - 3c_3}{6(1 - c_3)}, \quad b_3 = \frac{1}{6c_3(1 - c_3)}, \quad a_{31} = c_3^2, \quad a_{31} = c_3 - c_3^2.$$

It is also possible to use the highest order method to advance the solution. In this case, we still measure the local error estimate of the lowest order order solution, but we get a more accurate numerical solution for free. This idea is called *local extrapolation*.

MATLAB has two integrators based on explicit Runge-Kutta schemes, `ODE23` which is based on an order 3/2 pair by Bogacki and Shampine, (a 3th order advancing and a 2nd order error estimating method), and `ODE45` based on an order 5/4 pair by Dormand and Prince. Both use local extrapolation.

Stepsize control Let the user specify a tolerance Tol, and a norm $\|\cdot\|$ in which the error is measured. Let us start with t_n, y_n, and do one step forward in time with a stepsize h_n, giving y_{n+1} and le_{n+1}. If $\|le_{n+1}\| \leq Tol$ the step is accepted, and we proceed till the next step, maybe with an increased stepsize. If $\|le_{n+1}\| > Tol$ the step is rejected and we try again with a smaller stepsize. In both cases, we would like to find a stepsize h_{new} which gives a local error estimate smaller than Tol, but at the same time as close to Tol as possible. To find the right stepsize, we make one assumption: The function $\Psi(t_n, y_n)$ of the principle error term do not change much from one step to the next, thus $\|\Psi(t_n, y_n)\| \approx \|\Psi(t_{n+1}, y_{n+1})\| \approx C$. Then

$$\begin{array}{lll} \text{we have:} & \|le_{n+1}\| & \approx C \cdot h_n^{p+1} \\ \\ \text{we want:} & Tol & \approx C \cdot h_{new}^{p+1} \end{array}$$

We get rid of the unknown C by dividing the two equations with each other, and h_{new} can be solved from

$$\frac{\|le_{n+1}\|}{Tol} \approx \left(\frac{h_n}{h_{new}}\right)^{p+1}.$$

Rejected steps are wasted work, and it should be avoided. Thus we choose the new stepsize somewhat conservative. The new stepsize is computed by

$$h_{new} = P \cdot \left(\frac{Tol}{\|le_{n+1}\|}\right)^{\frac{1}{p+1}} h_n. \tag{14}$$

where P is a *pessimist factor*, usually chosen somewhere in the interval [0.5,0.95]. In the discussion so far we have used the requirement $\|le_{n+1}\| \leq Tol$, that is *error pr. step* (EPS). This do not take into account the fact that the smaller the step is, the more steps you take, and the local errors from each step adds up. From this point of view, it would make sense to rather use the requirement $le\|_{n+1} \leq Tol \cdot h_n$, that is *error pr. unit step* (EPUS). The stepsize selection is then given by

$$h_{new} = P \cdot \left(\frac{Tol}{\|le_{n+1}\|}\right)^{\frac{1}{p}} h_n. \tag{15}$$

Careful analysis has proved that the local extrapolation together with EPS gives proportionality between the global error and the tolerance. The same is true for the use of the lower order method to advance the solution in combination with EPUS.

5 Stiff equations and linear stability

Example 5.1. *Given the ODE*

$$y' = -1000y, \qquad y(0) = 1.$$

with exact solution

$$y(t) = e^{-1000t}.$$

Thus $y(t) \to 0$ as $t \to \infty$. The Euler method applied to this problem yields

$$y_{n+1} = y_n - 1000hy_n = (1 - 1000h)y_n.$$

so that $y_n = (1 - 1000h)^n$. This gives us two situations:

$$\begin{aligned} &\textit{If} \quad |1 - 1000h| < 1 \quad \textit{then} \quad y_n \to 0 \ \textit{as} \ n \to \infty. \\ &\textit{If} \quad |1 - 1000h| > 1 \quad \textit{then} \quad |y_n| \to \infty \ \textit{as} \ n \to \infty \end{aligned}$$

Clearly, the second situation does not make sense at all, as the numerical solution is unstable even if the exact solution is stable. We have to choose a stepsize $h < 0.002$ to get a stable numerical solution for this problem.

To be more general: Consider a linear ODE

$$y' = My, \qquad y(0) = y_0, \tag{16}$$

where M is a constant, $m \times m$ matrix. We assume that M is diagonalizable via an orthogonal transformation, that is

$$V^T M V = \Lambda$$

and $V^T V = V V^T = I$, where

$$\Lambda = diag\{\lambda_1, \lambda_2, \cdots, \lambda_m\}, \qquad V = [v_1, v_2, \cdots, v_m],$$

where λ_i, $i = 1, \cdots, m$ are the eigenvalues of M and v_i are the corresponding eigenvectors. By premultiplying (16) with V^T, we get

$$V^T y' = V^T M V V^T y, \qquad V^T y(t_0) = V^T y_0$$

or, using $u = V^T y$,

$$u' = \Lambda u, \qquad u(t_0) = V^T y_0 = u_0.$$

The system is now decoupled, and can be written componentwise as

$$u_i' = \lambda_i u_i, \qquad u_i(0) = u_{i,0}, \qquad \lambda_i \in \mathbb{C}, \qquad i = 1, \cdots, m. \tag{17}$$

We have to accept the possibility of complex eigenvalues, however, as M is a real matrix, then complex eigenvalues appear in complex conjugate pairs. In the following, we will consider the situation when

$$\mathrm{Re}(\lambda_i) < 0 \ \text{ for } \ i = 1, \cdots, m, \qquad \text{thus} \qquad u(t) \to 0 \text{ as } t \to \infty, \tag{18}$$

and $\|u(t)\|_2 \le \|u(0)\|_2$ for all $t > 0$. We obtain also

$$\|y\|_2 \le \|V\|_2 \|u\|_2,$$

and since $\|V\|_2 = 1$ we have also $\|y(t)\|_2 \le \|y_0\|_2$ for all $t > 0$ (the same observation can be obtained using another subordinate norm). The numerical solution is said to be stable when it reproduces the features of the exact solution and

$$\|y_n\|_2 \le \|y_0\|_2,$$

for $n = 1, 2, \ldots$.

Apply the Euler method to (16):

$$y_{n+1} = y_n + hMy_n.$$

We can do exactly the same linear transformations as above, so the system can be rewritten as

$$u_{i,n+1} = (1 + h\lambda_i) u_{i,n}, \qquad i = 1, \cdots, m.$$

For the numerical solution to be stable, we have to require

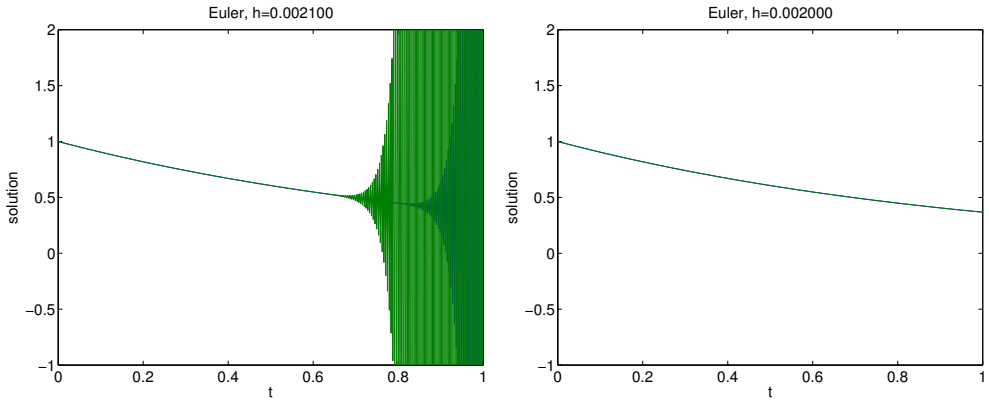
$$|1 + h\lambda_i| \le 1, \qquad \text{for all the eigenvalues } \lambda_i. \tag{19}$$

(The case $|1 + h\lambda_i h| = 1$ is included, as this is sufficient to prevent the solution from growing.)

Example 5.2. *Given*

$$y' = \begin{bmatrix} -2 & 1 \\ 998 & -999 \end{bmatrix} y, \qquad y(0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

with exact solution $y_1(t) = y_2(t) = e^{-t}$. *The matrix has eigenvalues* -1 *and* -1000. *The initial values are chosen so that the fast decaying mode is missing in the exact solution. This problem is solved by Eulers method, with two almost equal stepsizes,* $h = 0.0021$ *and* $h = 0.002$. *The difference is striking, the situation fits* (19) *and the result of Example 5.1. Note however that for this example* V *diagonalizing* M *is invertible but not orthogonal and* $\|V\|_2 \neq 1$ *so the analysis does not justify completely the behavior of the method.*



Example 5.2 is a typical example of a stiff equation. The stepsize is restricted by a fast decaying component. Stiffness occurs in situations with fast decaying solutions (transients) in combination with slow solutions. If you solve an ODE by an adaptive explicit scheme, and the stepsize becomes unreasonably small, stiffness is the most likely explanation. If the stepsizes in additions seems to be independent of your choice of tolerances, then you can be quite sure. The stepsize is restricted by stability related to the transients, and not by accuracy. The *backward Euler* method is one way to overcome this problem:

$$y_{n+1} = y_n + hf(t_{n+1}, y_{n+1}) \tag{20}$$

or, applied to the problem of (17)

$$u_{i,n+1} = u_{i,n} + h\lambda u_{i,n+1}, \qquad \Rightarrow \qquad u_{i,n+1} = \frac{1}{1 - h\lambda_i} u_{i,n}.$$

Since $|1/(1 - h\lambda_i)| \leq 1$ whenever $\mathrm{Re}(\lambda_i) \leq 0$ there is no stepsize restriction caused by stability issues. In fact, $u_{i,n+1} \to 0$ as $\mathrm{Re}(h\lambda_i) \to -\infty$, so fast transients decay quickly, as they are supposed to do. But this nice behaviour is not for free: for a nonlinear ODE a nonlinear system of equations has to be solved for each step. We will return to this topic later.

Linear stability theory for Runge-Kutta methods.

Given the linear test equation

$$y' = \lambda y, \qquad \lambda \in \mathbb{C}. \tag{21}$$

Thus $\lambda = \alpha + i\beta$. The solution can be expressed by

$$y(t_n + h) = e^{\alpha h} e^{i\beta h} y(t_n).$$

Clearly, the solution is stable if $\alpha \leq 0$, that is $\lambda \in \mathbb{C}^-$. For the numerical solution we then require the stepsize h to be chosen so that

$$|y_{n+1}| \leq |y_n| \quad \text{whenever} \lambda \in \mathbb{C}^- \tag{22}$$

When a RK method is applied (21), we simply get

$$y_{n+1} = R(z) y_n, \qquad z = h\lambda$$

where R is a polynomial or a rational function. R is called *the stability function* of the RK method. The numerical solution is stable if $|R(z)| \leq 1$, otherwise it is unstable. This motivates the following definition of *the region of absolute stability* as

$$\mathcal{D} = \{z \in \mathbb{C} \ : \ |R(z)| \leq 1\}.$$

The condition (22) is satisfied for all $h > 0$ if

$$\mathbb{C}^- \subseteq \mathcal{D},$$

Methods satisfying this condition are called *A-stable*. The Backward Euler method (20) is an example of an A-stable method.

Example 5.3. *A 2-stage ERK applied to* (21) *is given by:*

$$k_1 = \lambda y_n, \qquad k_2 = \lambda(y_n + h a_{21} \lambda y_n), \qquad y_{n+1} = y_n + h\lambda(b_1 + b_2) y_n + (h\lambda)^2 b_2 a_{21} y_n$$

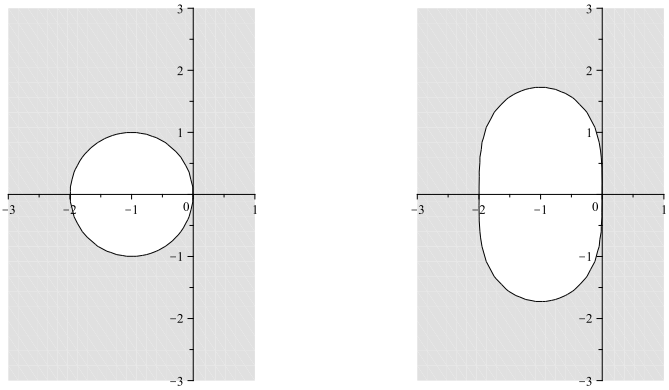
If this method is of order 2, then $b_1 + b_2 = 1$ *and* $b_2 a_{21} = 1/2$*, so that*

$$R(z) = 1 + z + \frac{1}{2} z^2.$$

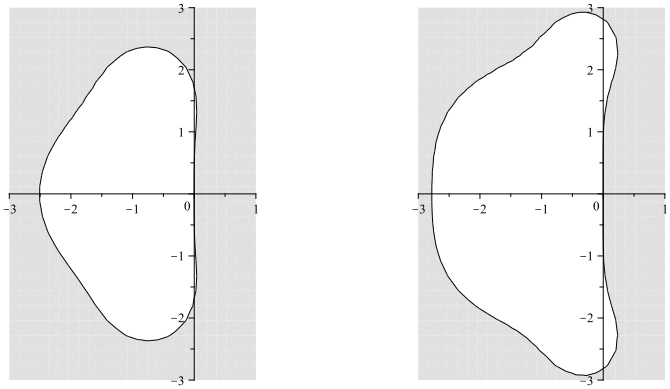
The stability function of an s-stage ERKs is a polynomial of degree s. As a consequence, no ERKs can be A-stable! If the order of the method is s, then

$$R(z) = \sum_{i=0}^{s} \frac{z^i}{i!}.$$

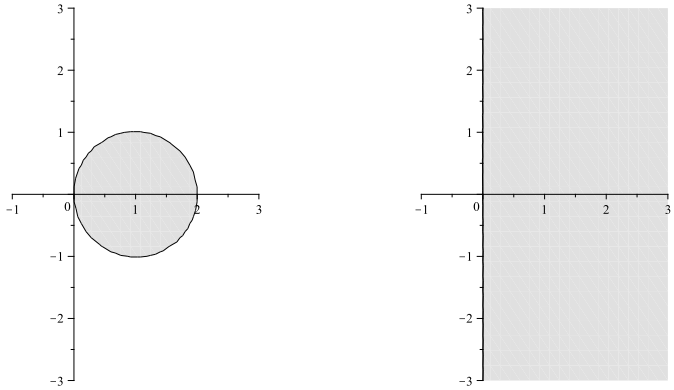
See Figure 3 for plots of the stability regions. But it has been proved that ERK with $p = s$ only exist for $s \leq 4$. To get an order 5 ERK, 6 stages are needed.



$p = s = 1$ $p = s = 2$



$p = s = 3$ $p = s = 4$



Backward Euler Trapezoidal rule

Figure 3: Stability regions in $\mathbb{C}^-$: The first four are the stability regions for explicit RK methods of order $p = s$. The white regions are stable, the grey unstable.

Example 5.4. *The trapezoidal rule (see section 3.1) applied to* (21) *gives*

$$y_{n+1} = y_n + \frac{h}{2}(\lambda y_n + \lambda y_{n+1}) \qquad \Rightarrow \qquad R(z) = \frac{1+z}{1-z}.$$

In this case $\mathcal{D} = \mathbb{C}^-$*, which is perfect.*

To summarise:

- For a given $\lambda \in \mathbb{C}^-$, choose a stepsize h so that $h\lambda \in \mathcal{D}$.
- If your problem is stiff, use an A-stable method.
- There are no A-stable explicit methods.

6 Linear multistep methods

A k-step linear multistep method (LMM) applied to the ODE

$$y' = f(t, y), \quad y(t_0) = y_0, \quad t_0 \le t \le t_{end}.$$

is given by

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = h \sum_{l=0}^{k} \beta_l f_{n+l}, \tag{23}$$

where α_l, β_l are the method coefficients, $f_j = f(t_j, y_j)$ and $t_j = t_0 + jh$, $h = (t_{end} - t_0)/Nstep$. Usually we require

$$\alpha_k = 1 \quad \text{and} \quad |\alpha_0| + |\beta_0| \neq 0.$$

To get started with a k-step method, we also need starting values $y_l \approx y(t_l)$, $l = 0, 1, \cdots, k-1$. A method is explicit if $\beta_k = 0$, otherwise implicit. The *leapfrog method*

$$y_{n+2} - y_n = 2hf(t_{n+1}, y_{n+1}) \tag{24}$$

and the method given by

$$y_{n+2} - y_{n+1} = h\left(\frac{3}{2}f_{n+1} - \frac{1}{2}f_n\right) \tag{25}$$

are both examples of explicit 2-step methods.

Example 6.1. *Given the problem*

$$y' = -2ty, \qquad y(0) = 1$$

with exact solution $y(t) = e^{-t^2}$. *Let* $h = 0.1$, *and* $y_1 = e^{-h^2}$. *This problem is solved by* (25), *and the numerical solution and the error is given by*

t_n	y_n	$\lvert e_n \rvert$
0.0	1.000000	0.00
0.1	0.990050	0.00
0.2	0.960348	$4.41 \cdot 10^{-4}$
0.3	0.912628	$1.30 \cdot 10^{-3}$
0.4	0.849698	$2.45 \cdot 10^{-3}$
0.5	0.775113	$3.69 \cdot 10^{-3}$
0.6	0.692834	$4.84 \cdot 10^{-3}$
0.7	0.606880	$5.75 \cdot 10^{-3}$
0.8	0.521005	$6.29 \cdot 10^{-3}$
0.9	0.438445	$6.41 \cdot 10^{-3}$
1.0	0.361746	$6.13 \cdot 10^{-3}$

The corresponding MATLAB code is given in `lmm.m`.

6.1 Consistency and order.

We define the *local discretization error* $\tau_{n+k}(h)$ by

$$h\tau_{n+k}(h) = \sum_{l=0}^{k} \left(\alpha_l y(t_{n+l}) - h\beta_l y'(t_{n+l}) \right). \tag{26}$$

You can think about the $h\tau_{n+k}$ as the defect obtained when plugging the exact solution into the difference equation (23). A method is *consistent* if $\tau_{n+k}(h) \underset{h\to 0}{\to} 0$. The term $h\tau_{n+k}(h)$ can be written as a power series in h

$$h\tau_{n+k}(h) = C_0 y(t_n) + C_1 h y'(t_n) + C_2 h^2 y''(t_n) + \cdots + C_q h^q y^{(q)}(t_n) + \cdots,$$

by expanding $y(t_n + lh)$ and $y'(t_n + lh)$ into their Taylor series around t_n,

$$y(t_n + lh) = y(t_n) + (lh)y'(t_n) + \frac{1}{2}(lh)^2 y''(t_n) + \cdots + \frac{(lh)^q}{q!} y^{(q)}(t_n) + \cdots$$
$$y'(t_n + lh) = y'(t_n) + (lh)y''(t_n) + \frac{1}{2}(lh)^2 y'''(t_n) + \cdots + \frac{(lh)^{q-1}}{q-1!} y^{(q)}(t_n) + \cdots$$

for sufficiently differentiable solutions $y(t)$. Insert this into (26), get the following expressions for C_q:

$$C_0 = \sum_{l=0}^{k} \alpha_l, \qquad C_q = \frac{1}{q!} \sum_{l=0}^{k} \left(l^q \alpha_l - q l^{q-1} \beta_l \right), \quad q = 1, 2, \cdots. \tag{27}$$

The method is consistent if $C_0 = C_1 = 0$. It is *of order p* if

$$C_0 = C_1 = \cdots = C_p = 0, \qquad C_{p+1} \neq 0.$$

The constant C_{p+1} is called the *error constant*.

Example 6.2. *The LMM* (25) *is defined by*

$$\alpha_0 = 0,\ \alpha_1 = -1,\ \alpha_2 = 1,\ \beta_0 = -\frac{1}{2},\ \beta_1 = \frac{3}{2},\ \beta_2 = 0,$$

thus

$$\begin{aligned}
C_0 &= \alpha_0 + \alpha_1 + \alpha_2 = 0. \\
C_1 &= \alpha_1 + 2\alpha_2 - (\beta_0 + \beta_1 + \beta_2) = 0 \\
C_2 &= \frac{1}{2!}\left(\alpha_1 + 2^2\alpha_2 - 2(\beta_1 + 2\beta_2)\right) = 0 \\
C_3 &= \frac{1}{3!}\left(\alpha_1 + 2^3\alpha_2 - 3(\beta_1 + 2^2\beta_2)\right) = \frac{5}{12}.
\end{aligned}$$

The method is consistent and of order 2.

Example 6.3. *Is it possible to construct an explicit 2-step method of order 3? There are 4 free coefficients $\alpha_0, \alpha_1, \beta_0, \beta_1$, and 4 order conditions to be solved ($C_0 = C_1 = C_2 = C_3 = 0$). The solution is*

$$\alpha_0 = -5,\ \alpha_1 = 4,\ \beta_0 = 2,\ \beta_1 = 4.$$

Test this method on the ODE of Example 2.1. (Replace the method coefficients in `lmm.m`*.) The result is nothing but disastrous. Taking smaller steps only increase the problem.*

To see why, you have to know a bit about how to solve difference equations.

6.2 Linear difference equations

A linear difference equation with constant coefficients is given by

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = \varphi_n, \qquad n = 0, 1, 2, \cdots . \tag{28}$$

The solution of this equation is a sequence $\{y_n\}$ of numbers (or vectors). Let $\{\tilde{y}_n\}$ be the general solution of the homogeneous problem

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = 0. \tag{29}$$

Let ψ_n be one particular solution of (28). The general solution of (28) is then $\{y_n\}$ where $y_n = \tilde{y}_n + \psi_n$. To find a unique solution, we will need the starting values $y_0, y_1, \cdots, y_{k-1}$.

Let us try $\tilde{y}_n = r^n$ as a solution of the homogeneous equation (29). This is true if

$$\sum_{l=0}^{k} \alpha_l r^{n+l} = r^n \sum_{l=0}^{k} \alpha_l r^l = 0.$$

The polynomial $\rho(r) = \sum_{l=0}^{k} \alpha_l r^l$ is called *the characteristic polynomial*, and $\{r^n\}$ is a solution of (29) if r is a root of $\rho(r)$. The kth degree polynomial $\rho(r)$ has k roots altogether, $r_1, r_2, \cdots, r_k$, they can be distinct and real, they can be distinct and complex, in which case they appear in complex conjugate pairs, or they can be multiple. In the latter case, say $r_1 = r_2 = \cdots = r_\mu$ we get a set of linear independent solutions $\{r_1^n\}$, $\{nr_1^n\}$, $\cdots$, $\{n^{\mu-1}r_1^n\}$. Altogether we have found k linear independent solutions $\{\tilde{y}_{n,l}\}$ of the homogeneous equation, and the general solution is given by

$$y_n = \sum_{l=1}^{k} \kappa_l \tilde{y}_{n,l} + \psi_n.$$

The coefficients κ_l can be determined from the starting values.

Example 6.4. *Given*

$$y_{n+4} - 6y_{n+3} + 14y_{n+2} - 16y_{n+1} + 8y_n = n$$
$$y_0 = 1,\ y_1 = 2,\ y_2 = 3\ y_3 = 4.$$

The characteristic polynomial is given by

$$\rho(r) = r^4 - 6r^3 + 14r^2 - 16r + 8$$

with roots $r_1 = r_2 = 2$, $r_3 = 1 + i$, $r_4 = 1 - i$. As a particular solution we try $\psi_n = an + b$. Inserted into the difference equation we find this to be a solution if $a = 1,\ b = 2$. The general solution has the form

$$y_n = \kappa_1 2^n + \kappa_2 n 2^n + \kappa_3 (1+i)^n + \kappa_4 (1-i)^n + n + 2.$$

From the starting values we find that $\kappa_1 = -1$, $\kappa_2 = \frac{1}{4}$, $\kappa_3 = -i/4$ and $\kappa_4 = i/4$. So, the solution of the problem is

$$\begin{aligned} y_n &= 2^n \left(\frac{n}{4} - 1\right) - \frac{i(1+i)^n}{4} + \frac{i(1-i)^n}{4} + n + 2 \\ &= 2^n \left(\frac{n}{4} - 1\right) - 2^{\frac{n-2}{2}} \sin\left(\frac{n\pi}{4}\right) + n + 2. \end{aligned}$$

Example 6.5. *The homogeneous part of the difference equation of Example 6.3 is*

$$\rho(r) = r^2 + 4r - 5 = (r-1)(r+5).$$

One root is 5. Thus, one solution component is multiplied by a factor -5 for each step, independent of the stepsize. Which explain why this method fails.

6.3 Zero-stability and convergence

Let us start with the definition of convergence. As before, we consider the error at t_{end}, using $Nstep$ steps with constant stepsize $h = (t_{end} - t_0)/Nstep$.

Definition 6.6.

- *A linear multistep method* (23) *is* convergent *if, for all ODEs satisfying the conditions of Theorem 2.4 we get*

  $$y_{Nstep} \underset{h\to 0}{\to} y(t_{end}), \qquad \textit{whenever} \qquad y_l \underset{h\to 0}{\to} y(t_0+lh), \quad l = 0, 1, \cdots, k-1.$$

- *The method is* convergent of order p *if, for all ODEs with f sufficiently differentiable, there exists a positive h_0 such that for all $h < h_0$*

  $$\|y(t_{end}-y_{Nstep}\| \le Kh^p \qquad \textit{whenever} \qquad \|y(t_0+lh)-y_l\| \le K_0 h^p, \quad l = 0, 1, \cdots, k-1.$$

The first characteristic polynomial of an LMM (23) is

$$\rho(r) = \sum_{l=0}^{k} \alpha_l r^l,$$

with roots $r_1, r_2, \cdots, r_k$. From the section on difference equation, it follows that for the boundedness of the solution y_n we require:

1. $|r_i| \le 1$, for $i = 1, 2, \cdots, k$.
2. $|r_i| < 1$ if r_i is a multiple root.

A method satisfying these two conditions is called *zero-stable*.

We can now state (without proof) the following important result:

Theorem 6.7. *(Dahlquist)*

$$\textit{Convergence} \qquad \Leftrightarrow \qquad \textit{Zero-stability + Consistency.}$$

For a consistent method, $C_0 = \sum_{l=0}^{k} \alpha_l = 0$ so the characteristic polynomial $\rho(r)$ will always have one root $r_1 = 1$.

The zero-stability requirement puts a severe restriction on the maximum order of a convergent k-step method:

Theorem 6.8. *(The first Dahlquist-barrier) The order p of a zero-stable k-step method satisfies*

$$\begin{aligned} p &\le k+2 \quad && \textit{if } k \textit{ is even,} \\ p &\le k+1 \quad && \textit{if } k \textit{ is odd,} \\ p &\le k \quad && \textit{if } \beta_k \le 0. \end{aligned}$$

Notice that the last line include all explicit LMMs.

6.4 Adams-Bashforth-Moulton methods

The most famous linear multistep methods are constructed by the means of interpolation. For instance by the following strategy:

The solution of the ODE satisfy the integral equation

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} f(t, y(t))dt. \tag{30}$$

Assume that we have found $f_i = f(t_i, y_i)$ for $i = n-k+1, \cdots, n$, with $t_i = t_0+ih$. Construct the polynomial of degree $k-1$, satisfying

$$p_{k-1}(t_i) = f(t_i, y_i), \qquad i = n-k+1, \ldots, n.$$

The interpolation points are equidistributed (constant stepsize), so Newton's backward difference formula can be used in this case (see Exercise 2), that is

$$p_{k-1}(t) = p_{k-1}(t_n + sh) = f_n + \sum_{j=1}^{k-1} (-1)^j \binom{-s}{j} \nabla^j f_n$$

where

$$(-1)^j \binom{-s}{j} = \frac{s(s+1)\cdots(s+j-1)}{j!}$$

and

$$\nabla^0 f_n = f_n, \qquad \nabla^j f_n = \nabla^{j-1} f_n - \nabla^{j-1} f_{n-1}.$$

Using $y_{n+1} \approx y(t_{n+1})$. $y_n \approx y(t_n)$ and $p_{k-1}(t) \approx f(t, y(t))$ in (30) gives

$$\begin{aligned} y_{n+1} - y_n \int_{t_n}^{t_{n+1}} p_{k-1}(t)dt &= h \int_0^1 p_{k-1}(t_n + sh)ds \\ &= hf_n + h \sum_{j=1}^{k-1} \left((-1)^j \int_0^1 \binom{-s}{1} ds \right) \nabla^j f_n. \end{aligned} \tag{31}$$

This gives the *Adams-Bashforth methods*

$$y_{n+1} - y_n = h \sum_{j=0}^{k-1} \gamma_j \nabla^j f_n, \qquad \gamma_0 = 1, \quad \gamma_j = (-1)^j \int_0^1 \binom{-s}{j} ds.$$

Example 6.9. *We get*

$$\gamma_0 = 1, \quad \gamma_1 = \int_0^1 s ds = \frac{1}{2}, \quad \gamma_2 = \int_0^1 \frac{s(s+1)}{2} ds = \frac{5}{12}$$

and the first few methods becomes:

$$\begin{aligned} y_{n+1} - y_n &= hf_n \\ y_{n+1} - y_n &= h\left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1} \right) \\ y_{n+1} - y_n &= h\left(\frac{23}{12} f_n - \frac{4}{3} f_{n-1} + \frac{5}{12} f_{n-1} \right) \end{aligned}$$

A k-step Adams-Bashforth method is explicit, has order k (which is the optimal order for explicit methods) and it is zero-stable. In addition, the error constant $C_{p+1} = \gamma_k$. Implicit Adams methods are constructed similarly, but in this case we include the (unknown) point (t_{n+1}, f_{n+1}) into the set of interpolation points. So the polynomial

$$p_k^*(t) = p_k^*(t_n + sh) = f_{n+1} + \sum_{j=1}^{k} (-1)^j \binom{-s+1}{j} \nabla^j f_{n+1}$$

interpolates the points (t_i, f_i), $i = n-k+1, \ldots, n+1$. Using this, we get the *Adams-Moulton* methods

$$y_{n+1} - y_n = h \sum_{j=0}^{k} \gamma_j^* \nabla^j f_{n+1}, \qquad \gamma_0^* = 1, \quad \gamma_j^* = (-1)^j \int_0^1 \binom{-s+1}{j} ds.$$

Example 6.10. *We get*

$$\gamma_0^* = 1, \quad \gamma_1^* = \int_0^1 (s-1) ds = -\frac{1}{2}, \quad \gamma_2^* = \int_0^1 \frac{(s-1)s}{2} ds = -\frac{1}{12}$$

and the first methods becomes

$$y_{n+1} - y_n = h f_{n+1} \qquad \textit{(Backward Euler)}$$

$$y_{n+1} - y_n = h \left(\frac{1}{2} f_{n+1} + \frac{1}{2} f_n \right) \qquad \textit{(Trapezoidal method)}$$

$$y_{n+1} - y_n = h \left(\frac{5}{12} f_{n+1} + \frac{2}{3} f_n - \frac{1}{12} f_{n-1} \right).$$

A k-step Adams-Moulton method is implicit, of order $k+1$ and is zero-stable. The error constant $C_{p+1} = \gamma_{k+1}^*$. Despite the fact that the Adams-Moulton methods are implicit, they have some advantages compared to their explicit counterparts: They are of one order higher, the error constants are much smaller, and the linear stability properties (when the methods are applied to the linear test problem $y' = \lambda y$) are much better.

k	0	1	2	3	4	5	6
γ_k	1	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\frac{19087}{60480}$
γ_k^*	1	$-\frac{1}{2}$	$-\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{19}{720}$	$-\frac{3}{160}$	$-\frac{863}{60480}$

Table 1: The γ's for the Adams methods.

6.5 Predictor-corrector methods

A predictor-corrector (PC) pair is a pair of one explicit (predictor) and one implicit (corrector) methods. The nonlinear equations from the application of the implicit method are solved by a fixed number of fixed point iterations, using the solution by the explicit method as starting values for the iterations.

Example 6.11. *We may construct a PC method from a second order Adams-Bashforth scheme and the trapezoidal rule as follows:*

$$
\begin{aligned}
&y_{n+1}^{[0]} = y_n + \frac{h}{2}(3f_n - f_{n-1}) && \textit{(P : Predictor)}\\
&\textit{for } l = 0, 1, \ldots, m\\
&\quad f_{n+1}^{[l]} = f(t_{n+1}, y_{n+1}^{[l]}) && \textit{(E : Evaluation)}\\
&\quad y_{n+1}^{[l+1]} = y_n + \frac{h}{2}(f_{n+1}^{[l]} + f_n) && \textit{(C : Corrector)}\\
&\textit{end}\\
&y_{n+1} = y_{n+1}^{[m]}\\
&f_{n+1} = f(t_{n+1}, y_{n+1}). && \textit{(E : Evaluation)}
\end{aligned}
$$

Such schemes are commonly referred as P(EC)^{m}E schemes.

The predictor and the corrector is often by the same order, in which case only one or two iterations are needed.

Error estimation in predictor-corrector methods.

The local discretization error of some LMM is given by

$$h\tau_{n+1} = \sum_{l=0}^{k}(\alpha_l y(t_{n-k+1+l} - h\beta_l y'(t_{n-k+1+l})) = h^{p+1}C_{p+1}y^{(p+1)}(t_{n-k+1}) + \mathcal{O}(h^{p+2}).$$

But we can do the Taylor expansions of y and y' around t_n rather than t_{n-k+1}. This will not alter the principal error term, but the terms hidden in the expression $\mathcal{O}(h^{p+2})$ will change. As a consequence, we get

$$h\tau_{n+1} = h^{p+1}C_{p+1}y^{(p+1)}(t_n) + \mathcal{O}(h^{p+2}).$$

Assume that $y_i = y(t_i)$ for $i = n-k+1, \ldots, n$, and $\alpha_k = 1$. Then

$$h\tau_{n+1} = y(t_{n+1}) - y_{n+1} + \mathcal{O}(h^{p+2}) = h^{p+1}C_{p+1}y^{(p+1)}(t_n) + \mathcal{O}(h^{p+2}).$$

Assume that we have chosen a predictor-corrector pair, using methods of the same order p. Then

$$
\begin{aligned}
&(P) && y(t_{n+1}) - y_{n+1}^{[0]} \approx h^{p+1}C_{p+1}^{[0]}y^{(p+1)}(t_n),\\
&(C) && y(t_{n+1}) - y_{n+1} \approx h^{p+1}C_{p+1}y^{(p+1)}(t_n),
\end{aligned}
$$

and

$$y_{n+1} - y_{n+1}^{[0]} \approx h^{p+1}(C_{p+1}^{[0]} - C_{p+1})y^{(p+1)}(t_n).$$

From this we get the following local error estimate for the corrector, called *Milne's device*:

$$y(t_{n+1}) - y_{n+1} \approx \frac{C_{p+1}}{C_{p+1]}^{[0]} - C_{p+1}}(y_{n+1} - y_{n+1}^{[0]}).$$

Example 6.12. *Consider the PC-scheme of Example 6.11. In this case*

$$C_{p+1}^{[0]} = \frac{5}{12}, \qquad C_{p+1} = -\frac{1}{12}, \qquad \textit{so} \qquad \frac{C_{p+1}}{C_{p+1]}^{[0]} - C_{p+1}} = -\frac{1}{6}.$$

Apply the scheme to the linear test problem

$$y' = -y, \qquad y(0) = 1,$$

using $y_0 = 1$, $y_1 = e^{-h}$ *and* $h = 0.1$. *One step of the PC-method gives*

l	$y_2^{[l]}$	$\lvert y_2 - y_2^{[l]}\rvert$	$\lvert y(0.2) - y_2^{[l]}\rvert$	$\frac{1}{6}\lvert y_2^{[l]} - y_2^{[0]}\rvert$
0	0.819112	$4.49 \cdot 10^{-4}$	$3.81 \cdot 10^{-4}$	
1	0.818640	$2.25 \cdot 10^{-5}$	$9.08 \cdot 10^{-5}$	$7.86 \cdot 10^{-5}$
2	0.818664	$1.12 \cdot 10^{-6}$	$6.72 \cdot 10^{-5}$	$7.47 \cdot 10^{-5}$
3	0.818662	$5.62 \cdot 10^{-8}$	$6.84 \cdot 10^{-5}$	$7.49 \cdot 10^{-5}$

After 1-2 iterations, the iteration error is much smaller than the local error, and we also observe that Milne's device gives a reasonable approximation to the error.

Remark Predictor-corrector methods are not suited for stiff problems. You can see this by e.g. using the trapezoidal rule on $y' = \lambda y$. The trapezoidal rule has excellent stability properties. But the iteration scheme

$$y_{n+1}^{[l+1]} = y_n + \frac{h}{2}\lambda(y_{n+1}^{[l]} + y_n)$$

will only converge if $|h\lambda/2| < 1$.

7 Orthogonal polynomials.

The aim of this section is to construct "optimal" quadrature formulas. To be more specific, given the integral

$$I_w(f) = \int_a^b w(x)f(x)dx \tag{32}$$

in which $w(x)$ is a fixed, positive function. We want to approximate this using a quadrature formula on the form

$$Q_w(f) = \sum_{i=0}^{n} A_i f(x_i).$$

Such a formula can be constructed as follows: Choose $n+1$ distinct nodes, $x_0, x_1, \cdots, x_n$ in the interval $[a, b]$. Construct the interpolation polynomial

$$p_n(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x), \qquad \ell_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

An approximation to the integral is then given by

$$Q_w(f) = \int_a^b w(x)p_{n-1}(x)dx = \sum_{i=0}^{m} A_i f(x_i), \qquad A_i = \int_a^b w(x)\ell_i(x)dx. \quad (33)$$

The quadrature formula is of precision m if

$$I_w(p) = Q_w(p), \qquad \text{for all } p \in \mathbb{P}_m.$$

From the construction, these quadrature formulas is of precision at least n. The question is how too choose the nodes x_i, $i = 0, \ldots, n$ giving m as large as possible. The key concept here is *orthogonal polynomials*.

Orthogonal polynomials.

Given two functions $f, g \in C[a, b]$. We define an inner product of these two functions by

$$< f, g >= \int_a^b w(x)f(x)g(x)dx, \qquad w(x) > 0. \quad (34)$$

Thus the definition of the inner product depends on the integration interval $[a, b]$ and a given *weight function* $w(x)$. If $f, g, h \in C[a, b]$ and $\alpha \in \mathbb{R}$ then

$$\begin{aligned} \langle f, g\rangle_w &= \langle g, f\rangle_w \\ \langle f + g, h\rangle_w &= \langle f, h\rangle_w + \langle g, h\rangle_w \\ \langle \alpha f, g\rangle_w &= \alpha\langle f, g\rangle_w \\ \langle f, f\rangle_w \geq 0, \qquad &\text{and} \qquad \langle f, f\rangle_w = 0 \Leftrightarrow f \equiv 0. \end{aligned}$$

From an inner product, we can also define a norm on $C[a, b]$ by

$$\|f\|_w^2 = \langle f, f\rangle_w.$$

For the inner product (34) we also have

$$\langle xf, g\rangle_w = \int_a^b w(x)xf(x)g(x)dx = \langle f, xg\rangle_w. \quad (35)$$

Our aim is now to create an orthogonal basis for $\mathbb{P}$, that is, create a sequence of polynomials $\phi_k(x)$ of degree k (no more, no less) for $k = 0, 1, 2, 3, \ldots$ such that

$$\langle \phi_i, \phi_j\rangle_w = 0 \quad \text{for all} \quad i \neq j.$$

If we can make such a sequence, then

$$\mathbb{P}_{n-1} = \text{span}\{\phi_0, \phi_1, \cdots, \phi_{n-1}\} \qquad \text{and} \qquad \langle \phi_n, p\rangle_w = 0 \quad \text{for all} \qquad p \in \mathbb{P}_{n-1}.$$

Let us now find the sequence of orthogonal polynomials. This is done by a Gram-Schmidt process:

Let $\phi_0 = 1$. Let $\phi_1 = x - B_1$ where B_1 is given by the orthogonality condition:

$$0 = \langle \phi_1, \phi_0 \rangle_w = \langle x, 1 \rangle_w - B_1 \langle 1, 1 \rangle_w \qquad \Rightarrow \qquad B_1 = \frac{\langle x, 1 \rangle_w}{\|1\|_w^2}.$$

Let us now assume that we have found ϕ_j, $j = 0, 1, \ldots, k-1$. Then, let

$$\phi_k = x\phi_{k-1} - \sum_{j=0}^{k-1} \alpha_j \phi_j.$$

Clearly, ϕ_k is a polynomial of degree k, and α_j can be chosen so that $\langle \phi_k, \phi_i \rangle_w = 0$, $i = 0, 1, \ldots, k-1$, or

$$\langle \phi_k, \phi_i \rangle_w = \langle x\phi_{k-1}, \phi_i \rangle_w - \sum_{j=0}^{k-1} \alpha_j \langle \phi_i, \phi_j \rangle_w = \langle x\phi_{k-1}, \phi_i \rangle_w - \alpha_i \langle \phi_i, \phi_i \rangle_w = 0, \qquad i = 0, 1, \cdots, k-1.$$

So $\alpha_i = \langle x\phi_{k-1}, \phi_i \rangle_w / \langle \phi_i, \phi_i \rangle_w$. But we can do even better. Since ϕ_{k-1} is orthogonal to all polynomials of degree $k-2$ or less, we get

$$\langle x\phi_{k-1}, \phi_i \rangle_w = \langle \phi_{k-1}, x\phi_i \rangle_w = 0 \quad \text{for} \quad i + 1 < k - 1.$$

So, we are left only with α_{k-1} and α_{k-2}. The following theorem concludes the argument:

Theorem 7.1. *The sequence of orthogonal polynomials can be defined as follows:*

$$\begin{aligned} &\phi_0(x) = 1, \qquad \phi_1(x) = x - B_1 \\ &\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k \phi_{k-2}(x), \qquad k \geq 2 \end{aligned}$$

with

$$B_k = \frac{\langle x\phi_{k-1}, \phi_{k-1} \rangle_w}{\|\phi_{k-1}\|_w^2}, \qquad C_k = \frac{\langle x\phi_{k-1}, \phi_{k-2} \rangle_w}{\|\phi_{k-2}\|_w^2} = \frac{\|\phi_{k-1}\|_w^2}{\|\phi_{k-2}\|_w^2}$$

The last simplification of C_k is given by:

$$\begin{aligned} \langle x\phi_{k-1}, \phi_{k-2} \rangle_w &= \langle \phi_{k-1}, x\phi_{k-2} \rangle_w \\ \phi_{k-1} &= x\phi_{k-2} - B_{k-1}\phi_{k-2} - C_{k-1}\phi_{k-3}. \end{aligned}$$

Solve the second with respect to $x\phi_{k-2}$, replace it into the right hand side of the first expression, and use the orthogonality conditions.

Example 7.2. *For the inner product*

$$\langle f, g \rangle = \int_{-1}^{1} f(x) g(x) dx$$

we get

$$\begin{aligned}
&\phi_0 = 1, && \langle x\phi_0, \phi_0\rangle = 0, && \langle \phi_0, \phi_0\rangle = 2, && B_1 = 0, && \\
&\phi_1 = x, && \langle x\phi_1, \phi_1\rangle = 0, && \langle \phi_1, \phi_1\rangle = \frac{2}{3}, && B_2 = 0, && C_2 = \frac{1}{3} \\
&\phi_2 = x^2 - \frac{1}{3} && \langle x\phi_2, \phi_2\rangle = 0, && \langle \phi_2, \phi_2\rangle = \frac{8}{45}, && B_3 = 0, && C_3 = \frac{4}{15} \\
&\phi_3 = x^3 - \frac{3}{5}x, && \textit{etc.}
\end{aligned}$$

These are the well known Legendre polynomials.

Example 7.3. *Let* $w(x) = 1/\sqrt{1-x^2}$*, and* $[a, b] = [-1, 1]$*. We then get the sequence of polynomials:*

$$\begin{aligned}
&\phi_0 = 1, && \langle x\phi_0, \phi_0\rangle_w = 0, && \langle \phi_0, \phi_0\rangle_w = \pi, && B_1 = 0, && \\
&\phi_1 = x, && \langle x\phi_1, \phi_1\rangle_w = 0, && \langle \phi_1, \phi_1\rangle_w = \frac{\pi}{2}, && B_2 = 0, && C_2 = \frac{1}{2} \\
&\phi_2 = x^2 - \frac{1}{2} && \langle x\phi_2, \phi_2\rangle_w = 0, && \langle \phi_2, \phi_2\rangle_w = \frac{\pi}{2}, && B_3 = 0, && C_3 = \frac{1}{4} \\
&\phi_3 = x^3 - \frac{3}{4}x, && \textit{etc.}
\end{aligned}$$

These are nothing but the monic Chebyshev polynomials $\tilde{T}_k$*.*

The following theorem will become useful:

Theorem 7.4. *Let* $f \in C[a, b]$*,* $f \not\equiv 0$ *satisfying* $\langle f, p\rangle_w = 0$ *for all* $p \in P_{k-1}$*. Then* f *changes signs at least* k *times on* (a, b)*.*

Proof. By contradiction. Suppose that f changes sign only $r < k$ times, at the points $t_1 < t_2 < \cdots < t_r$. Then f will not change sign on each of the subintervals:

$$(a, t_1), (t_1, t_2), \cdots, (t_{r-1}, t_r), (t_r, b).$$

Let $p(x) = \prod_{i=1}^{r}(x - t_i) \in \mathbb{P}_r \subseteq \mathbb{P}_{k-1}$. Then $p(x)$ has the same sign properties as $f(x)$, and $f(x)p(x)$ does not change sign on the interval. Since $w > 0$ we get

$$\int_a^b w(x)f(x)p(x) \neq 0$$

which contradicts the assumption of the theorem. □

Corollary 7.5. *The orthogonal polynomial* ϕ_k *has exactly* k *distinct zeros in* (a, b)*.*

8 Solution of systems of nonlinear equations

Given a system of nonlinear equations

$$F(x) = 0, \qquad F : \mathbb{R}^m \to \mathbb{R}^m \tag{36}$$

for which we assume that there is (at least) one solution $x^\star$. The idea is to rewrite this system into the form

$$x = G(x), \qquad G : \mathbb{R}^m \to \mathbb{R}^m. \tag{37}$$

The solution $x^\star$ of (36) should satisfy $x^\star = G(x^\star)$, and is thus called a *fixed point* of G. The iteration schemes becomes: given an initial guess $x^{(0)}$, the *fixed point iterations* becomes

$$x^{(k+1)} = G(x^{(k)}), \qquad k = 1, 2, \dots . \tag{38}$$

The following questions arise:

(i) How to find a suitable function G?
(ii) Under what conditions will the sequence $x^{(k)}$ converge to the fixed point $x^\star$?
(iii) How quickly will the sequence $x^{(k)}$ converge?

Point (ii) can be answered by Banach fixed point theorem:

Theorem 8.1. *Let $D \subseteq \mathbb{R}^m$ be a convex*[2] *and closed*[3] *set. If*

$$G(D) \subseteq D \tag{39a}$$

and

$$\|G(y) - G(v)\| \le L\|y - v\|, \qquad \text{with } L < 1 \text{ for all } y, v \in D, \tag{39b}$$

then G has a unique fixed point in D and the fixed point iterations (38) *converges for all $x^{(0)} \in D$. Further,*

$$\|x^{(k)} - x^\star\| \le \frac{L^k}{1 - L}\|x^{(1)} - x^{(0)}\|. \tag{39c}$$

Proof. The proof is based on the *Cauchy Convergence theorem*, saying that a sequence $\{x^{(k)}\}_{k=0}^{\infty}$ in $\mathbf{R}^m$ converges to some $x^\star$ if and only if for every $\varepsilon > 0$ there is an N such that

$$\|x^{(l)} - x^{(k)}\| < \varepsilon \qquad \text{for all} \quad l, k > N. \tag{40}$$

Assumption (39a) ensures $x^{(k)} \in D$ as long as $x^{(0)} \in D$. From (38) and (39b) we get:

$$\|x^{(k+1)} - x^{(k)}\| = \|G(x^{(k)}) - G(x^{(k-1)})\| \le L\|x^{(k)} - x^{(k-1)}\| \le L^k\|x^{(1)} - x^{(0)}\|.$$

We can write $x^{(k+p)} - x^{(k)} = \sum_{i=1}^{p}(x^{(k+i)} - x^{(k+i-1)})$, thus

$$\begin{aligned}\|x^{(k+p)} - x^{(k)}\| &\le \sum_{i=1}^{p}\|x^{(k+i)} - x^{(k+i-1)}\| \\ &\le (L^{p-1} + L^{p-2} + \cdots + 1)\|x^{(k+1)} - x^{(k)}\| \le \frac{L^k}{1 - L}\|x^{(1)} - x^{(0)}\|,\end{aligned}$$

[2] D is convex if $\theta y + (1 - \theta)v \in D$ for all $y, v \in D$ and $\theta \in [0, 1]$.

[3] A set $D \in \mathbf{R}^m$ is closed if it contains all its *limit points*. A limit point of D is $x \in \mathbf{R}^m$ such that for all neighborhoods J_x of x, $J_x \cap D \neq \emptyset$.

since $L < 1$. For the same reason, the sequence satisfy (40), so the sequence converges to some $x^\star \in D$. Since the inequality is true for all $p > 0$ it is also true for $x^\star$, proving (39c).

To prove that the fixed point is unique, let $x^\star$ and $y^\star$ be two different fixed points in D. Then

$$\|x^\star - y^\star\| = \|G(x^\star) - G(y^\star)\| < \|x^\star - y^\star\|$$

which is impossible. □

For a given problem, it is not necessarily straightforward to justify the two assumptions of the theorem. But it is sufficient to find some L satisfying the condition $L < 1$ in some norm to prove convergence.

Let $x = [x_1, \ldots, x_m]^T$ and $G(x) = [g_1(x), \ldots, g_m(x)]^T$. Let $y, v \in D$, and let $x(\theta) = \theta y + (1-\theta)v$ be the straight line between y and v. The mean value theorem for functions gives

$$\begin{aligned} g_i(y) - g_i(v) = g_i(x(1)) - g_i(x(0)) &= \frac{dg_i}{d\theta}(\tilde{\theta})(1-0), \qquad \tilde{\theta} \in (0,1) \\ &= \sum_{j=1}^{m} \frac{\partial g_i}{\partial x_j}(\tilde{x}_i)(y_j - v_j), \qquad \tilde{x}_i = \tilde{\theta} y + (1-\tilde{\theta})v \end{aligned}$$

since $dx_j(\theta)/d\theta = y_j - v_j$. Then

$$|g_i(y) - g_i(v)| \le \sum_{j=1}^{m} |\frac{\partial g_i}{\partial x_j}(\tilde{x}_i)| \cdot |y_j - v_j| \le \left(\sum_{j=1}^{m} |\frac{\partial g_i}{\partial x_j}(\tilde{x}_i)| \right) \max_l |y_l - v_l|.$$

If we let $\bar{g}_{ij}$ be some upper bound for each of the partial derivatives, that is

$$|\frac{\partial g_i}{\partial x_j}(x)| \le \bar{g}_{ij}, \quad \text{for all } x \in D.$$

then

$$\|G(y) - G(v)\|_\infty = \left(\max_i \sum_{j=1}^{m} \bar{g}_{ij} \right) \|y - v\|_\infty.$$

We can then conclude that (39b) is satisfied if

$$\max_i \sum_{j=1}^{m} \bar{g}_{ij} < 1.$$

Newton's method

Newton's method is a fixed point iterations for which

$$G(x^{(k)}) = x^{(k)} - J(x^{(k)})^{-1} F(x^{(k)}),$$

where the *Jacobian* is the matrix function

$$J(x) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x) & \cdots & \frac{\partial f_1}{\partial x_m}(x) \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1}(x) & \cdots & \frac{\partial f_m}{\partial x_m}(x) \end{pmatrix}.$$

It is possible to prove that if *i)* (36) has a solution $x^\star$, *ii)* $J(x)$ is nonsingular in some open neighbourhood around $x^\star$ and *iii)* the initial guess $x^{(0)}$ is sufficiently close to $x^\star$, the Newton iterations will converge to $x^\star$ and

$$\|x^\star - x^{(k+1)}\| \leq K\|x^\star - x^{(k)}\|^2$$

for some positive constant K. We say that the convergence is *quadratic*.

Steepest descent

Steepest descent is an algorithm that search for a (local) minimum of a given function $g : \mathbb{R}^m \to \mathbb{R}$. The idea is as follows.
a) Given some point $x \in \mathbb{R}^m$.
b) Find the direction of steepest decline of g from x (steepest descent direction)
c) Walk steady in this direction till g starts to increase again.
d) Repeat from a).

The direction of steepest descent is $-\nabla g(x)$, where the gradient ∇g is given by

$$\nabla g(x) = \left[\frac{\partial g}{\partial x_1}(x), \ldots, \frac{\partial g}{\partial x_m}(x)\right]^T.$$

And the steepest descent algorithm reads

function STEEPEST DESCENT(g, $x^{(0)}$)
  for k=0,1,2,.... **do**
    $z = -\nabla g(x^{(k)})/\|\nabla g(x^{(k)})\|$ ▷ The steepest descent direction.
    Minimize $g(x^{(k)} + \alpha z)$, giving $\alpha = \alpha^\star$.
    $x^{(k+1)} = x^{(k)} + \alpha^\star z$
  end for
end function

This algorithm will always converge to some point $x^\star$ in which $\nabla g(x^\star) = 0$, usually a local minimum, if one exist. But the convergence can be very slow.

This can be used to find solution of the nonlinear system of equations (36) by defining

$$g(x) = F(x)^T F(x) = \|F(x)\|_2^2.$$

Thus, $x^\star$ is a minimum of $g(x)$ if and only if $x^\star$ is a solution of $F(x) = 0$. In this case, we can show that

$$\nabla g(x) = 2J(x)^T F(x).$$

9 Bernoulli polynomials and the Euler-Maclaurin formula.

Let the integral

$$I(f) = \int_a^b f(x)dx$$

be approximated by the Trapezoidal rule

$$T(h) = h\left(\frac{1}{2}f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}f(x_n)\right)$$

where $x_i = a + ih$, $i = 0, \cdots, n$ with $h = (b-a)/n$. The aim of this note is to prove that the error can be written as

$$I(f) - T(h) = \sum_{k=1}^{m-1} \frac{b_{2k}}{(2k)!} h^{2k}(f^{(2k-1)}(a) - f^{(2k-1)}(b)) - \frac{b_{2m}}{(2m)!} h^{2m}(b-a)\, f^{(2m)}(\eta) \tag{41}$$

where $\eta \in (a,b)$, and b_k are the Bernoulli numbers. These will be defined later. Obviously, the formula requires $f \in C^{2m}[a,b]$. The formula proves that the error can be written as an even power series of h, which is the theoretical fundament for the development of the Romberg integration algorithm.

We will first define the well known Bernoulli polynomials which will then be used to prove Euler-Maclaurin's formula. This again will be used to prove (41).

Bernoulli polynomials.

For our purpose, it is convenient to define the Bernoulli polynomials by the following reccurence relation:

$$\begin{aligned} &B_0(t) = 1, \\ &B_k'(t) = kB_{k-1}(t) \quad \text{and} \quad \int_0^1 B_k(t) = 0, \qquad k \geq 1. \end{aligned}$$

The first few polynomials become

$$\begin{aligned} B_1(t) &= t - \frac{1}{2} \\ B_2(t) &= t^2 - t + 1/6 \\ B_3(t) &= t^3 - \frac{3}{2}t^2 + \frac{1}{2}t. \end{aligned}$$

We will need the following properties of these polynomials:

$$B_k(0) = B_k(1), \qquad k \geq 2, \tag{42a}$$

$$B_k(1-t) = (-1)^k B_k(t), \tag{42b}$$

$$B_k(t) - B_k(0) \qquad \text{has no zeros in (0,1) if } k \text{ is even.} \tag{42c}$$

The *Bernoulli numbers* are given by $b_k = B_k(0)$. As a consequence of (42a) and (42b) we get $b_k = 0$ for k odd and $k \geq 3$. The Bernoulli numbers can also be found by the generating function

$$\frac{t}{e^t - 1} = \sum_{k=0}^{\infty} \frac{b_k}{k!} t^k.$$

Euler-Maclaurin's formula

By repeated use of integration by parts and the Bernoulli polynomials, we get

$$\begin{aligned}
\int_0^1 f(t)dt &= \int_0^1 f(t)B_0(t)dt \\
&= f(t)B_1(t)\Big|_0^1 - \int_0^1 B_1(t)f'(t)dt \\
&= \frac{1}{2}[f(1) + f(0)] - \frac{1}{2}B_2(t)f'(t)\Big|_0^1 + \frac{1}{2}\int_0^1 B_2(t)f''(t)dt \\
&= \frac{1}{2}[f(1) + f(0)] - \sum_{j=2}^{\bar{m}} \frac{(-1)^j}{j!} B_j(t)f^{(j-1)}(t)\Big|_0^1 + (-1)^{\bar{m}} \frac{1}{\bar{m}!}\int_0^1 B_n(t)f^{(n)}(t)dt.
\end{aligned}$$

Now, since $B_{2k+1}(0) = B_{2k+1}(1) = 0$ and $B_{2k}(0) = B_{2k}(1) = b_{2k}$ this can be written as

$$\begin{aligned}
\int_0^1 f(t)dt = \frac{1}{2}[f(1) + f(0)] &- \sum_{k=1}^{m-1} \frac{b_{2k}}{(2k)!}\big[f^{(2k-1)}(1) - f^{(2k-1)}(0)\big] \\
&- \frac{b_{2m}}{(2m)!}\big[f^{(2m-1)}(1) - f^{(2m-1)}(0)\big] + \frac{1}{(2m)!}\int_0^1 B_{2m}(t)f^{(2m)}(t)dt.
\end{aligned}$$

Using property (42c) and the mean value theorem for integrals, the last two terms become

$$-\frac{1}{(2m)!}\int_0^1 \big[b_{2m} - B_{2m}(t)\big]f^{(2m)}(t)dt = -\frac{b_{2m}}{(2m)!}f^{(2m)}(\eta).$$

As a result, we get the *Euler-Maclaurin formula*:

$$\int_0^1 f(t)dt = \frac{1}{2}[f(1)+f(0)] - \sum_{k=1}^{m-1} \frac{b_{2k}}{(2k)!}\big[f^{(2k-1)}(1) - f^{(2k-1)}(0)\big] - \frac{b_{2m}}{(2m)!}f^{(2m)}(\eta).$$

Error of the Trapezoidal rule.

Applying the Euler-Maclaurin formula to a function $g(t) = f(x_i + ht)$, using the change of variables $t = (x - x_i)/h$ gives

$$\begin{aligned}
\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}[f(x_i) + f(x_{i+1})] &- \sum_{k=1}^{m-1} \frac{b_{2k}}{(2k)!}h^{2k}\big[f^{(2k-1)}(x_{i+1}) - f^{(2k-1)}(x_i)\big] \\
&- \frac{b_{2m}}{(2m)!}h^{2m}f^{(2m)}(\eta_i).
\end{aligned}$$

The expression (41) is finally obtained by summing over all the intervals $[x_i, x_{i+1}]$.

10 Linear algebra: introduction

We consider the approximation of the solution of linear systems of algebraic equations with n equations and n unknowns:

$$\begin{array}{rcl} a_{1,1}x_1 + a_{1,2}x_2 + \cdots + a_{1,n}x_n &=& b_1 \\ a_{2,1}x_1 + a_{2,2}x_2 + \cdots + a_{2,n}x_n &=& b_2 \\ \vdots & \vdots & \vdots \\ a_{n,1}x_1 + a_{n,2}x_2 + \cdots + a_{n,n}x_n &=& b_n \end{array} \tag{43}$$

where $(x_1, \cdots, x_n)$ are the unknowns. Given $(a_{i,j})_{1\le i,j\le n}$, and b_i, $i = 1, \cdots, n$.

We can rewrite (43) in a matrix form by defining:

$$A := \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & \cdots & a_{2,n} \\ \vdots & \vdots & \cdots & \cdots & \vdots \\ a_{n,1} & a_{n,2} & \cdots & \cdots & a_{n,n} \end{bmatrix}, \quad x := \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad b := \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

so we have that (43) becomes

$$A \cdot x = b. \tag{44}$$

Linear systems can be easily solved when A has a special structure, for example when A is a diagonal matrix or triangular matrix and $a_{i,i} \neq 0$ for $i = 1, \ldots, n$:

- A diagonal matrix

$$A = \begin{bmatrix} a_{1,1} & 0 & \cdots & \cdots & 0 \\ 0 & a_{2,2} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \cdots & a_{n,n} \end{bmatrix} \Rightarrow \begin{array}{rcl|rcl} a_{1,1}x_1 &=& b_1 & x_1 &=& \frac{b_1}{a_{1,1}} \\ a_{2,2}x_2 &=& b_2 & x_2 &=& \frac{b_2}{a_{2,2}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n,n}x_n &=& b_n & x_n &=& \frac{b_n}{a_{n,n}} \end{array}$$

- A triangular matrix

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & \cdots & a_{1,n} \\ 0 & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & 0 & a_{n-1,n-1} & a_{n-1,n} \\ 0 & 0 & \cdots & 0 & a_{n,n} \end{bmatrix} \Rightarrow$$

$$
\begin{array}{rcccl}
a_{1,1}x_1 + a_{1,2}x_2 + \cdots + \cdots + a_{1,n}x_n & = & b_1 & & \\
a_{2,2}x_2 + \cdots + \cdots + a_{2,n}x_n & = & b_2 & & \\
\cdots & \vdots & \vdots & \Rightarrow & \\
a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n & = & b_{n-1} & & \\
a_{n,n}x_n & = & b_n & &
\end{array}
$$

$$
\begin{array}{rcc}
x_1 & = & \frac{b_1 - \sum_{j=2}^{n} a_{1,j}x_j}{a_{1,1}} \\
x_2 & = & \frac{b_2 - \sum_{j=3}^{n} a_{2,j}x_j}{a_{2,2}} \\
\vdots & \vdots & \vdots \\
x_{n-1} & = & \frac{b_{n-1} - a_{n-1,n}x_n}{a_{n-1,n-1}} \\
x_n & = & \frac{b_n}{a_{n,n}}
\end{array}
\qquad (45)
$$

The formula (45) is called back substitution algorithm. For general maurices other techniques based on matrix factorizations are in general used. If the matrix is of large size and *sparse* (i.e. it has a relatively small number of elements different from zero), then it is more convenient to use iterative techniques. We will describe here briefly both approaches. In the next section we consider the stability of linear systems, that is the sensitivity of the output with respect to perturbations in the input data.

11 Stability of linear systems

11.1 Preliminaries

A vector norm is a function $\|\cdot\| : \mathbf{R}^n \to \mathbf{R}$ satisfying three axioms:

1. $\|u\| \geq 0$ for all $u \in \mathbf{R}^n$ and $\|u\| = 0$ if and only if $u = 0$.
2. $\|\lambda u\| = |\lambda|\|u\|$for all vectors $u \in \mathbf{R}^n$ and scalars $\lambda \in \mathbf{R}$.
3. $\|u + v\| \leq \|u\| + \|v\|$ for all $u \in \mathbf{R}^n$ and $v \in \mathbf{R}^n$.

If u is a vector with n components, examples of norms are:

- $\|u\|_1 := |u_1| + \cdots + |u_n|$, norm-1;
- $\|u\|_\infty := \max_{1 \leq i \leq n} |u_i|$, max-norm;

- $\|u\|_2 := \left(|u_1|^2 + \cdots + |u_n|^2\right)^{\frac{1}{2}} = \left(u^T u\right)^{\frac{1}{2}}$, norm-2.

We will also make use of matrix-norms. Matrix-norms satisfy an extra axiom compared to vector norms; this axiom has to do with the product of matrices, so if A and B are $n \times n$ matrices, for a vector-norm according to this axiom we have that

$$\|AB\| \leq \|A\|\|B\|.$$

Assume U is a matrix with elements $u_{i,j}$, examples of matrix-norms are:

- $\|U\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^n u_{i,j}^2}$, Frobenius norm;
- $\|U\|_\infty := \max_i \sum_{j=1}^n |u_{i,j}|$ max-norm;
- $\|U\|_1 := \max_j \sum_{i=1}^n |u_{i,j}|$ norm-1.

For example for

$$U := \begin{bmatrix} 3 & 2 \\ -1 & 0 \end{bmatrix},$$

we get

$$\begin{aligned} \|U\|_F &= \sqrt{3^2 + 2^2 + (-1)^2} = \sqrt{14} = 3.74165738677394, \\ \|U\|_\infty &= \max\{|3| + |2|, |-1| + |0|\} = 5, \\ \|U\|_1 &= \max\{|3| + |-1|, |2| + |0|\} = 4. \end{aligned}$$

11.2 Stability analysis

Consider $Ax = b$, A invertible. Let $x(\varepsilon)$ be the solution of the linear system

$$(A + \varepsilon F)x(\varepsilon) = (b + \varepsilon f).$$

We are intersted in the case when ε tends to zero. Here $f \in \mathbf{R}^n$ and F is $n \times n$ matrix.

We seek for bounds for the relative error

$$\frac{\|x - x(\varepsilon)\|}{\|x\|},$$

for a chosen vector-norm $\|\cdot\|$. We will also make use of the so called subordinate matrix-norm deduced from $\|\cdot\|$, that is for a given $n \times n$ matrix B:

$$\|B\| := \max_{x \neq 0,\, x \in \mathbf{R}^n} \frac{\|Bx\|}{\|x\|}.$$

Proposition 11.1. *Assume A is invertible. For all ε such that $\varepsilon \leq C_\varepsilon$, $A + \varepsilon F$ is also invertible.*

Proposition 11.2. *For all ε such that $\varepsilon \leq \tilde{C}_\varepsilon$, here exists a unique $x(\varepsilon)$ and its components, $x_i(\varepsilon)$ are continuous functions of ε.*

Lemma 11.3.

$$\frac{d}{d\varepsilon}x(\varepsilon)\bigg|_{\varepsilon=0} = A^{-1}(f - Fx).$$

Proof. By differentiation.

We now use Taylor theorem and obtain

$$x(\varepsilon) = x(0) + \varepsilon x'(0) + \mathcal{O}(\varepsilon^2),$$

where $x(0) = x$. So

$$\|x(\varepsilon) - x\| \leq \varepsilon\|x'(0)\| + \mathcal{O}(\varepsilon^2),$$

and using the lemma, we obtain

$$\|x(\varepsilon) - x\| \leq \varepsilon\|A^{-1}(f - Fx)\| + \mathcal{O}(\varepsilon^2).$$

This leads to

$$\frac{\|x(\varepsilon) - x\|}{\|x\|} \leq \varepsilon\frac{\|A^{-1}(f - Fx)\|}{\|x\|} + \mathcal{O}(\varepsilon^2) \leq \varepsilon\|A^{-1}\|\left(\frac{\|f\|}{\|x\|} + \frac{\|Fx\|}{\|x\|}\right) + \mathcal{O}(\varepsilon^2).$$

Now $Ax = b$ implies $\|b\| \leq \|A\|\|x\|$, and this is equivalent to

$$\frac{1}{\|x\|} \leq \frac{\|A\|}{\|b\|}.$$

We also have

$$\frac{\|Fx\|}{\|x\|} \leq \|F\| = \frac{\|F\|\|A\|}{\|A\|}.$$

So proceeding in the estimation of the relative error we get

$$\frac{\|x(\varepsilon) - x\|}{\|x\|} \leq \varepsilon\|A^{-1}\|\left(\frac{\|f\|\|A\|}{\|b\|} + \frac{\|F\|\|A\|}{\|A\|}\right) + \mathcal{O}(\varepsilon^2),$$

and we obtain

$$\frac{\|x(\varepsilon) - x\|}{\|x\|} \leq \varepsilon\|A^{-1}\|\|A\|\left(\frac{\|f\|}{\|b\|} + \frac{\|F\|}{\|b\|}\right) + \mathcal{O}(\varepsilon^2).$$

The real number

$$\mathcal{K}(A) := \|A^{-1}\|\,\|A\|$$

is called **condition number** of A. The condition number depends on A and on the matrix-norm used to measure the relative error. The final bound of the relative error is then

$$\frac{\|x(\varepsilon) - x\|}{\|x\|} \leq \varepsilon\,\mathcal{K}(A)\left(\frac{\|f\|}{\|b\|} + \frac{\|F\|}{\|b\|}\right) + \mathcal{O}(\varepsilon^2),$$

and we clearly see that the condition number gives a bound of the leading error term (in ε) of the relative error in the output data by means of the relative error in the input data.

We observe that since $I = A^{-1}A$, then

$$\|I\| \leq \|A^{-1}\| \, \|A\| = \mathcal{K}(A),$$

and for all subordinate matrix-norms

$$\|I\| = \max_{x \neq 0,\, x \in \mathbf{R}^n} \frac{\|I\, x\|}{\|x\|} = 1,$$

so

$$1 \leq \mathcal{K}(A).$$

12 Gaussian elimination

Definition. Two linear systems of equations are said to be equivalent if they have the same solution.

Gaussian elimination is an algorithm where in $n-1$ steps, $Ax = b$ is transformed in an equivalent system $Ux = f$ and U is an upper triangular matrix. The advantage is that triangular systems can be easily solved using the formula (45).

In particular we have

$$Ax = b \to A^{(1)}x = b^{(1)} \to \cdots \to A^{(k)}x = b^{(k)} \to \cdots \to A^{(n-1)}x = b^{(n-1)}$$

all intermediate linear systems $A^{(k)}x = b^{(k)}$ $k = 1, \ldots, n-1$ are equivalent to $Ax = b$. The last system $A^{(n-1)}x = b^{(n-1)}$, is in upper triangular form, and system number k is

$$A^{(k)} = \begin{bmatrix} \tilde{a}_{1,1} & \cdots & \tilde{a}_{1,k} & \tilde{a}_{1,k+1} & \cdots & \tilde{a}_{1,n} \\ 0 & \ddots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \ddots & \tilde{a}_{k,k} & \tilde{a}_{k,k+1} & \cdots & \tilde{a}_{k,n} \\ \vdots & \vdots & 0 & \tilde{a}_{k+1,k+1} & \cdots & \tilde{a}_{k+1,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & \tilde{a}_{n,k+1} & \cdots & \tilde{a}_{n,n} \end{bmatrix}.$$

We obtain $A^{(1)}x = b^{(1)}$ from $Ax = b$ by replacing the den 2nd, 3rd, .., nth equation in $Ax = b$ with corresponding linear combinations of the first equation with the 2nd, 3rd, .., nth equation. To obtain $A^{(2)}x = b^{(2)}$ (and the subsequent linear systems) the same process is repeated considering only prosessen er repetert med å ta hensyn til kolonnene fra the columns form the 2nd to the nth and the rows from the 2nd to the nth.

12.1 Example

Given:

$$\begin{array}{rcl} x_1 + 4x_2 + x_3 &=& 6 \\ 2x_1 - x_2 - 2x_3 &=& 3 \\ x_1 + 3x_2 + 2x_3 &=& 5 \end{array} \qquad A = \begin{bmatrix} 1 & 4 & 1 \\ 2 & -1 & -2 \\ 1 & 3 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 3 \\ 5 \end{bmatrix} \tag{46}$$

we want to reduce it t a triangular form.

We start with replacing the second equation with a linear combination of the first two equations, that is we replace
$2x_1 - x_2 - 2x_3 = 3$ with

$$(2x_1 - x_2 - 2x_3) + (-2) \cdot (x_1 + 4x_2 + x_3) = 3 + (-2) \cdot 6, \Rightarrow -9x_2 - 4x_3 = -9.$$

We then replace the 3rd equation with a linear combination of the 3rd and 1st equation:

$$(x_1 + 3x_2 + 2x_3) + (-1) \cdot (x_1 + 4x_2 - x_3) = 5 + (-1) \cdot 6, \Rightarrow -x_2 + x_3 = -1.$$

This way we get the following new system

$$\begin{array}{rcl} x_1 + 4x_2 + x_3 &=& 6 \\ -9x_2 - 4x_3 &=& -9 \\ -x_2 + x_3 &=& -1 \end{array} \qquad A^{(1)} = \begin{bmatrix} 1 & 4 & 1 \\ 0 & -9 & -4 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -9 \\ -1 \end{bmatrix} \tag{47}$$

The coefficients used in the linear combination of the equations are $\begin{bmatrix} 2 \\ 1 \end{bmatrix}$, and they are chosen so that in the new system we get that the second and third element of the first column vanish, this way we *eliminate* to coefficients in the linear system.

Now we work only with the two last equations:

$$\begin{array}{rcl} -9x_2 - 4x_3 &=& -9 \\ -x_2 + x_3 &=& -1 \end{array} \tag{48}$$

We replace the last equaltion with

$$(-x_2 + x_3) + (-\frac{1}{9}) \cdot (-9x_2 - 4x_3) = -1 + \left(-\frac{1}{9}\right) \cdot (-9) \Rightarrow \frac{13}{9} x_3 = 0.$$

The coefficient used for the linear combination is $\frac{1}{9}$.

In the end we get the linear system

$$\begin{array}{rcl} x_1 + 4x_2 + x_3 &=& 6 \\ -9x_2 - 4x_3 &=& -9 \\ \frac{13}{9} x_3 &=& 0 \end{array} \qquad A^{(2)} = \begin{bmatrix} 1 & 4 & 1 \\ 0 & -9 & -4 \\ 0 & 0 & \frac{13}{9} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -9 \\ 0 \end{bmatrix} \tag{49}$$

and the solution can be computed by the backward substitution algorithm. Starting form the last equation $x_3 = 0$, and proceeding upwards to solve $-9x_2 = -9 \Rightarrow x_2 = 1$ og $x_1 + 4 = 6 \Rightarrow x_1 = 2$, we get

$$x = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}.$$

Note now that when we *eliminated* the first column we used the two coefficients:

$$\begin{bmatrix} 2 \\ 1 \end{bmatrix},$$

and for the second we used

$$\frac{1}{9}.$$

By using these coefficients we construct a triangular matrix L:

$$L := \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & \frac{1}{9} & 1 \end{bmatrix}.$$

Note also that if from (49) we define now $U := A^{(2)}$ and we compute $L \cdot U$, we get A back.

In general when we perform the Gaussian elimination, we compute simultaneously a factorization of the matrix $A = LU$, where L and U are two triangular matrices.

This is very handy if we want to compute solution of two or more systems with the same coefficient matrix A but different right hand sides, b, $\hat{b}$ and so on. In this case one can use the same factorization $LU = A$ two (or more) times ganger and compute to different backward substitutions, one with b and one with $\hat{b}$.

Such factorization is also used for computing the determinant of A, because $\det(A) = \prod_{i=1}^{n} u_{i,i}$. Analogously one can use the factorization to find the inverse A^{-1}. In our case we have

$$\det(A) = 1 \cdot (-9) \cdot \frac{13}{9} = -13$$

and

$$A^{-1} = \begin{bmatrix} 1 & 4 & 1 \\ 0 & -9 & -4 \\ 0 & 0 & \frac{13}{9} \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & \frac{1}{9} & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & \frac{4}{9} & \frac{7}{13} \\ 0 & -\frac{1}{9} & -\frac{4}{13} \\ 0 & 0 & \frac{9}{13} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -\frac{7}{9} & -\frac{1}{9} & 1 \end{bmatrix}$$

Note that it is much easier to compute the inverse of a triangular matrix than the inverse of a general invertible but unstructured matrix.

12.2 Gauss elimination: general algorithm

For the general matrix (43) we have:

$$Ax = b \to A^{(1)}x = b^{(1)}$$

if $a_{1,1} \neq 0$

$$\left.\begin{array}{lllllll} l_{2,1} := \frac{a_{2,1}}{a_{1,1}} & a_{2,p}^{(1)} := a_{2,p} - l_{2,1}a_{1,p} & b_2^{(1)} := b_2 - l_{2,1}b_1 \\ l_{3,1} := \frac{a_{3,1}}{a_{1,1}} & a_{3,p}^{(1)} := a_{3,p} - l_{3,1}a_{1,p} & b_3^{(1)} := b_3 - l_{3,1}b_1 \\ \vdots & & \\ l_{n,1} := \frac{a_{n,1}}{a_{1,1}} & a_{n,p}^{(1)} := a_{n,p} - l_{n,1}a_{1,p} & b_n^{(1)} := b_n - l_{n,1}b_1 \end{array}\right\} p = 2, \ldots, n.$$

Now we define

$$A := A^{(1)}, b := b^{(1)}$$

and continue with

$$Ax = b \to A^{(2)}x = b^{(2)}.$$

If $a_{2,2} \neq 0$, we obtain, for $j = 3, \ldots, n$,

$$l_{j,2} := \frac{a_{j,2}}{a_{2,2}} \quad a_{j,p}^{(2)} := a_{j,p} - l_{j,2}a_{2,p} \quad b_j^{(2)} := b_j - l_{j,2}b_2 \quad p = 3, \ldots, n,$$

and then we define

$$A := A^{(2)}, b := b^{(2)}.$$

In general for $A^{(k)}$ we have,

$$A := A^{(k-1)}, b := b^{(k-1)}$$

and

$$Ax = b \to A^{(k)}x = b^{(k)}$$

with

$$l_{j,k} := \frac{a_{j,k}}{a_{k,k}} \quad a_{j,p}^{(k)} := a_{j,p} - l_{j,k}a_{k,p} \quad b_j^{(k)} := b_j - l_{j,k}b_k \quad p = k+1, \ldots, n.$$

for $j = k+1, \ldots n$, and assuming $a_{k,k} \neq 0$. In the end we obtain the following algorithm:

Gaussian elimination

For $k = 1, \ldots, n-1$

For $j = k+1, \ldots, n$

$l_{j,k} := \frac{a_{j,k}}{a_{k,k}}$

For $p = k+1, \ldots, n+1,$

$a_{j,p} := a_{j,p} - l_{j,k} a_{k,p}$

End

End

End

And with $U := A^{(n-1)}$ we also obtain the following, so called LU**-factorization** for A,

$$A = LU.$$

12.3 Gaussian elimination with partial pivoting

In Gaussisan elimination (G-E), as described on the general algorithm, we divide always by $a_{k,k}$ (the so called pivot element). Obviously we might get problems when such value is zero or very small. To avoid such problems we can perform systematic permutationns of the rows of the linear system. This procedure is called partial pivoting.

12.4 Two exmples: Gaussian elimination with partial pivoting

Consider the linear system

$$\begin{array}{rcl} x_1 + x_2 + x_3 + x_4 &=& 1 \\ x_1 + x_2 + 2x_3 - x_4 &=& 1 \\ x_1 + 2x_2 - x_3 - x_4 &=& 1 \\ x_1 - x_2 + x_3 - x_4 &=& 1 \end{array} \qquad \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & -1 \\ 1 & 2 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{array}\right] \tag{50}$$

We eliminate the first column by subtracting the first row from the other three. We obtain

$$\begin{array}{rcl} x_1 + x_2 + x_3 + x_4 &=& 1 \\ x_3 - 2x_4 &=& 0 \\ x_2 - 2x_3 - 2x_4 &=& 0 \\ -2x_2 - 2x_4 &=& 0 \end{array} \qquad \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & -2 \\ 0 & 1 & -2 & -2 \\ 0 & -2 & 0 & -2 \end{array}\right] \tag{51}$$

now we can not proceede, because there is no α which could be used to eliminate x_2

$$(x_2 - 2x_3 - 2x_4) - \alpha \cdot (x_3 - 2x_4) = 0.$$

The only option is to permute the rows. To minimize roundoff error propagation it pays off to exchange the second row with the row having the biggest coefficient in absolute value for x_2, that is the third. Then we get

$$\begin{array}{rcl} x_1 + x_2 + x_3 + x_4 &=& 1 \\ -2x_2 - 2x_4 &=& 0 \\ x_2 - 2x_3 - 2x_4 &=& 0 \\ x_3 - 2x_4 &=& 0 \end{array} \qquad \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & -2 \\ 0 & 1 & -2 & -2 \\ 0 & 0 & 1 & -2 \end{array}\right] \tag{52}$$

and now we continue the Gaussian elimination as usual. We obtain:

$$\begin{array}{rcl} x_1 + x_2 + x_3 + x_4 &=& 1 \\ -2x_2 - 2x_4 &=& 0 \\ -2x_3 - 3x_4 &=& 0 \\ x_3 - 2x_4 &=& 0 \end{array} \qquad \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & -2 \\ 0 & 0 & -2 & -3 \\ 0 & 0 & 1 & -2 \end{array}\right] \tag{53}$$

and in the end:

$$\begin{array}{rcl} x_1 + x_2 + x_3 + x_4 &=& 1 \\ -2x_2 - 2x_4 &=& 0 \\ -2x_3 - 3x_4 &=& 0 \\ -\frac{7}{2}x_4 &=& 0 \end{array} \qquad \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & -2 \\ 0 & 0 & -2 & -3 \\ 0 & 0 & 0 & -\frac{7}{2} \end{array}\right] \tag{54}$$

which, by the backward substitution algorithm, gives the following solution

$$x = \left[\begin{array}{c} 1 \\ 0 \\ 0 \\ 0 \end{array}\right].$$

In the second example given:

$$\begin{aligned} x_1 + 3x_2 + 2x_3 &= 5 \\ 2x_1 - x_2 - 2x_3 &= 3 \\ x_1 + 4x_2 + x_3 &= 6 \end{aligned} \qquad A = \begin{bmatrix} 1 & 3 & 2 \\ 2 & -1 & -2 \\ 1 & 4 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ 6 \end{bmatrix} \tag{55}$$

we want to reduce the system to triangular form using Gaussian elimination with partial pivoting.

We exchange rows:

$$\begin{aligned} 2x_1 - x_2 - 2x_3 &= 3 \\ x_1 + 3x_2 + 2x_3 &= 5 \\ x_1 + 4x_2 + x_3 &= 6 \end{aligned} \tag{56}$$

then we eliminate x_1,

$$\begin{aligned} 2x_1 - x_2 - 2x_3 &= 3 \\ 3.5x_2 + 3x_3 &= 3.5 \\ 4.5x_2 + 2x_3 &= 4.5 \end{aligned} \tag{57}$$

we exchange rows once more:

$$\begin{aligned} 2x_1 - x_2 - 2x_3 &= 3 \\ 4.5x_2 + 2x_3 &= 4.5 \\ 3.5x_2 + 3x_3 &= 3.5 \end{aligned} \tag{58}$$

and eliminate x_2 from the last equation,

$$\begin{aligned} 2x_1 - x_2 - 2x_3 &= 3 \\ 4.5x_2 + 2x_3 &= 4.5 \\ 1.4444x_3 &= 0 \end{aligned} \tag{59}$$

with the backward substitution algorithm we obtain the solution $x_3 = 0$, $x_2 = 1$, $x_1 = 2$.

12.5 G-E with partial pivoting: general algorithm

In general we get the following Gaussian elimination algorithm with partial pivoting: first one initializes the vector π (pivot vektor) so that $\pi_i := i$ for $i = 1, \ldots n$,

Gaussian elimination with partial pivoting

For $k = 1, \ldots, n-1$

$a := |a_{k,k}|$

  For $j = k+1, \ldots, n$

    if ($a < |a_{j,k}|$)

      $a := |a_{j,k}|$

      $\pi_k := j$

    End

  End

  if ($\pi_k \neq k$)

    $s := \pi_k$

    For $p = k, \ldots, n$

      $r := a_{k,p}$

      $a_{k,p} := a_{s,p}$

      $a_{s,p} := r$

    End

  End

  For $j = k+1, \ldots, n$

    $l_{j,k} := \frac{a_{j,k}}{a_{k,k}}$

    For $p = k+1, \ldots, n+1$,

      $a_{j,p} := a_{j,p} - l_{j,k} a_{k,p}$

    End

  End

End

12.6 Complexity of Gaussian elimination

One can prove that for a $n \times n$ matrix the complexity of Gaussian elimination is of

$$\frac{1}{3}n^3 - \frac{1}{3}n,$$

operations (additions and multiplications). For big n $\frac{1}{3}n^3$ dominates the cost. We say that Gaussian elimination has complexity $\mathcal{O}(n^3)$. The backward substitution algorithm, (45)) has lower cost, that is $\mathcal{O}(n^2)$.

13 Other matrix factorizations

Bisides the LU-factorizations there are many other important matrix factorizations which is useful to know about.

Recall that an eigenvalue of A is a real or complex value such that, there is u vector such that

$$Au = \lambda u.$$

u is called eigenvector of A.

1. QR**- factorization**: any real matrix A $n \times p$ can be factorized in the form

   $$A = QR$$

   where Q is $n \times n$ orthogonal (i.e. $Q^TQ = QQ^T = I$ where I is the identity matrix) and R is $n \times p$ is upper triangular.

2. **Polar decomposition**: any matrix A $n \times n$ can be factorized in the form

   $$A = QS$$

   where Q is $n \times n$ orthogonal and S is $n \times n$ is symmetric.

3. **Schur canonical form**: for any matrix A $n \times n$ there exists a matrix P (complex) unitary (i.e. $P^HP = PP^H = I$ and P^H the transpose-conjugate of P) such that

   $$P^HAP = T$$

   where T is upper triangular.

   As a consequence, if A is Hermitian (i.e. $A = A^H$) then

   $$P^HAP = P^HA^HP = T$$

   and T is Hermitian and triangular and therefore is diagonal.

4. **Singular value decomposition**. For all A $n \times n$ real matrices, A can be factorized as

   $$A = U\Sigma V^T$$

   where Σ is diagonal, U and V are $n \times n$ orthogonal matrices. The diagonal elements of Σ are the singular values of A, i.e. the square roots of the eigenvalues of A^TA. This factorization has analogs for $n \times p$ matrices and for matrices with complex entries.

5. **Jordan canonical form**. For any A real $n \times n$ (or $A \in \mathbb{C}^{n\times n}$) it exists a matrix $M \in \mathbb{C}^{n\times n}$ invertible, such that

$$M^{-1}AM = J = \begin{bmatrix} J_1 & & & \\ & J_2 & & \\ & & \ddots & \\ & & & J_k \end{bmatrix}, \qquad \text{(block-diagonal)}. \tag{60}$$

Here J_i is a $m_i \times m_i$-matrix, and $\sum_{i=1}^{k} m_i = n$. The *Jordan-blocks* J_i have the form

$$J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix}, \quad \text{if } m_i \geq 2$$

and $J_i = [\lambda_i]$ if $m_i = 1$. If all $m_i = 1$, then $k = n$ and the matrix is diagonalizable. If A has n distinct egenvalues, it is always diagonalizable. The converse is not true, that is a matrix can be diagonalizable even if it has multiple eigenvalues.

14 Symmetric matrices

When we talk about symmetric matrices, we mean normally *real* symmetric matrices. The *transpose* A^T of a $m \times n$-matrix A, is a $n \times m$-matrix with a_{ji} as the (ij)-element (a matrix whose columns are the rows of A). A $n \times n$ matrix is symmetric if $A^T = A$.

A symmetric $n \times n$ matrix has real eigenvalues $\lambda_1, \ldots, \lambda_n$ and a set of real orthonormal eigenvectors $x_1, \ldots, x_n$. Let $\langle \cdot, \cdot \rangle$ denote the standard inner-product on $\mathbb{C}^n$, then $\langle x_i, x_j \rangle = \delta_{ij}$ (Kronecker-delta).

A consequence of this is that the matrix of eigenvectors $X = [x_1, \ldots, x_n]$ is real and orthogonal and its inverse is therefore the transpose

$$X^{-1} = X^T.$$

The diagonalization of A is given by

$$\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n), \quad X = [x_1, \ldots, x_n], \quad X^T X = I, \quad X^T A X = \Lambda \Leftrightarrow A = X \Lambda X^T$$

14.1 Positive definite matrices

If A is symmetric and $\langle x, Ax \rangle = x^T Ax > 0$ for all $0 \neq x \in \mathbb{R}^n$ A is called *positive definite*. Here we denote with $\langle \cdot, \cdot \rangle$ the Euclidean inner product.

A (symmetric) is positive semi-definite if $\langle x, Ax \rangle \geq 0$ for all $x \in \mathbb{R}^n$ and $\langle x, Ax \rangle = 0$ for at least a $x \neq 0$.

A positive definite $\Leftrightarrow$ A has only positive eigenvalues.

A positive semi-definite $\Leftrightarrow$ A has only non-negative eigenvalues, and at least a 0-eigenvalue.

15 Gershgorin's theorem

Gershgorin's theorem. Is given $A = (a_{ik}) \in \mathbb{C}^{n\times n}$. Define n disks S_j in the complex plane by

$$S_j = \left\{ z \in \mathbb{C} : |z - a_{jj}| \leq \sum_{k\neq j} |a_{jk}| \right\}.$$

The union $S = \bigcup_{j=1}^{n} S_j$ contains all the eigenvalues of A. For every eigenvalue λ of A there is a j such that $\lambda \in S_j$.
Example.

$$A = \begin{bmatrix} 1+i & 1 & 0 \\ 0.5 & 3 & 1 \\ 1 & 1 & 5 \end{bmatrix}.$$

□

Proof of Gershgorin's theorem: Let λ be a eigenvalue with associate eigenvector $x = [\xi_1, \ldots, \xi_n]^T \neq 0$. Choose ℓ among the indexes $1, \ldots, n$ such that $|\xi_\ell| \geq |\xi_k|,\ k = 1, \ldots, n$, and so $|\xi_\ell| > 0$. The equation $Ax = \lambda x$ has component ℓ:

$$\sum_{k=1}^{n} a_{\ell k}\xi_k = \lambda\,\xi_\ell \ \Rightarrow\ (\lambda - a_{\ell\ell})\xi_\ell = \sum_{k\neq\ell} a_{\ell k}\xi_k$$

Divide by $|\xi_\ell|$ on each side and take the absolute value

$$|\lambda - a_{\ell\ell}| \quad = \quad \left| \sum_{k\neq\ell} a_{\ell k}\frac{\xi_k}{\xi_\ell} \right| \quad \leq \quad \sum_{k\neq\ell} |a_{\ell k}|\frac{|\xi_k|}{|\xi_\ell|} \quad \leq \quad \sum_{k\neq\ell} |a_{\ell k}|$$

Then we get $\lambda \in S_\ell$.

Example. Diagonally dominant matrices with positive diagonal elements are positive definite. Why?

16 Solution of linear systems by iteration

To approximate x in the numerical solution of $Ax = b$, given $x^{(0)}$, we construct a sequence of vectors $x^{(1)}, \ldots, x^{(n)}, \ldots$. A way to do this is by fixed-point iteration.

We consider an equivalent formulation of $Ax = b$ as fix-point equaltion. For example:

$$Ax = b \Leftrightarrow x = (I - A)x + b$$

where I is the $n \times n$ identity matrix. Given x_0, we then obtain the iteration:

$$x^{(n+1)} = (I - A)x^{(n)} + b.$$

In general one can obtain an iteration as follows:

- write A as a sum of two terms: $A = M - N$, choose M invertible;
- from $(M - N)x = b$ one gets $Mx = Nx + b$ and

$$x = M^{-1}Nx + M^{-1}b;$$

- so given x^0 one builds the iteration:

$$x^{(n+1)} = M^{-1}Nx^{(n)} + M^{-1}b.$$

Typically M is chosen such that M^{-1} is easy to compute, for example M can be diagonal or triangular.

16.1 Example

We want to solve with fix-point-iteration the system

$$\begin{array}{rcl} x_1 - x_2 & = & 1 \\ -x_1 + 2x_2 & = & -1 \end{array} \quad A := \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \tag{61}$$

and start with

$$x^{(0)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The solution is

$$x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

We take

$$M := \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad N = M - A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

We have $Mx = Nx + b$, and $x = M^{-1}Nx + M^{-1}b$, i.e.

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

By using $x^{(0)}$ we compute

$$x^{(1)} = M^{-1}Nx^{(0)} + M^{-1}b,$$

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 1 \\ -\frac{1}{2} \end{bmatrix}.$$

We continue $x^{(2)} = M^{-1}Nx^{(1)} + M^{-1}b$:

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} + \begin{bmatrix} 1 \\ -\frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix}$$

and more

$$\begin{bmatrix} x_1^{(3)} \\ x_2^{(3)} \end{bmatrix} = \begin{bmatrix} 1 \\ -0.2500 \end{bmatrix}, \quad \begin{bmatrix} x_1^{(4)} \\ x_2^{(4)} \end{bmatrix} = \begin{bmatrix} 0.7500 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} x_1^{(5)} \\ x_2^{(5)} \end{bmatrix} = \begin{bmatrix} 1 \\ -0.1250 \end{bmatrix},$$

$$\begin{bmatrix} x_1^{(6)} \\ x_2^{(6)} \end{bmatrix} = \begin{bmatrix} 0.8750 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} x_1^{(28)} \\ x_2^{(28)} \end{bmatrix} = \begin{bmatrix} 1.0000 \\ -0.0000 \end{bmatrix}.$$

16.2 Example

In the system (61) we take

$$M := \begin{bmatrix} 1 & 0 \\ -1 & 2 \end{bmatrix} \qquad N = M - A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},$$

and with the same $x^{(0)}$ we compute $x^{(1)} = M^{-1}Nx^{(0)} + M^{-1}b$:

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

and we get the true solution of the system already at the first iteration.

In general if M is the diagonal part of A, i.e.

$$m_{i,i} = a_{i,i}, \quad i = 1, \ldots, n, \quad m_{i,j} = 0, \quad i \neq j,$$

(where $m_{i,j}$ are the elements of M, and $a_{i,j}$ are the elements of A), then we obtain the so called **Jacobi method**.

If M is the lower triangular part of A, i.e.

$$m_{i,j} = a_{i,j}, \quad i = 1, \ldots, n, \; j = 1, \ldots, i, \quad m_{i,j} = 0, \quad i = 1, \ldots, n, \; j = i{+}1, \ldots, n,$$

then the method is called **Gauss-Seidel method**.

16.3 Convergence

To measure the extent to which x^n has converged to x we use vector norms: $\|x - x^{(n)}\|$.

We write the iteration in the following general way

$$x^{(n+1)} = M^{-1}Nx^{(n)} + M^{-1}b,$$

by defining $C := M^{-1}N$ and $g := M^{-1}b$ we can write:

$$x^{(n+1)} = Cx^{(n)} + g. \tag{62}$$

Theorem 16.1. *If there is a matrix-norm $\|\cdot\|$ such that $\|C\| < 1$ the iteration (62) converges for all $x^{(0)}$.*

16.4 Example

Consider

$$B = \begin{bmatrix} 3 & 1 \\ -1 & 2.5 \end{bmatrix}, M = \begin{bmatrix} 3 & 0 \\ 0 & 2.5 \end{bmatrix}, N = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

then

$$C_J = M^{-1}N = \begin{bmatrix} 0 & -0.3333 \\ 0.4000 & 0 \end{bmatrix}$$

and $\|C_J\|_F = 0.5207$, $\|C_J\|_1 = \|C_J\|_{\max} = 0.4000$, so given f, the Jacobi method converges for $Bx = f$ for any $x^{(0)}$.

For the Gauss-Seidel method we have

$$C_{GS} = \begin{bmatrix} 3 & 0 \\ -1 & 2.5 \end{bmatrix}^{-1} \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -0.3333 \\ 0 & -0.1333 \end{bmatrix}$$

and $\|C_{GS}\|_F = 0.3590$, $\|C_{GS}\|_1 = 0.4667$ and $\|C_{GS}\|_{\max} = 0.3333$, so Gauss-Seidel method converges for $Bx = f$ and for any $x^{(0)}$.

16.5 Example

Consider the matrix from the example (61):

$$A := \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix},$$

Both Jacobi and Gauss-Seidel converge. For the Jacobi method we have:

$$C_J = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \frac{1}{2} & 0 \end{bmatrix}$$

with norms $\|C_J\|_F \geq 1$ $\|C_J\|_{\max} \geq 1$ $\|C_J\|_1 \geq 1$. For Gauss-Seidel

$$C_{GS} = \begin{bmatrix} 1 & 0 \\ -1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & \frac{1}{2} \end{bmatrix}$$

and $\|C_{GS}\|_F \geq 1$ $\|C_{GS}\|_{\max} \geq 1$ $\|C_{GS}\|_1 \geq 1$.

Here the hypothesis of the previous theorem are not satisfied, even if in our numerical experiments the iteration converges. We should use another technique to prove convergence. Let $\sigma(C)$ be the set of eigenvalues of C, then we can define

$$\rho(C) := \max_{\lambda \in \sigma(C)} |\lambda|$$

$\rho(C)$ is named spectral radius of C, and it is a positive number.

One can show that

Theorem 16.2. *$\rho(C) < 1$ if and only if the iterative method (62) converges for all $x^{(0)}$.*

In our example we must look at the eigenvalues of C_J and C_{GS}. Note that

$$Cu = \lambda u \Leftrightarrow (C - \lambda I)u = 0 \Leftrightarrow \det(C - \lambda I) = 0,$$

where I is the identity matrix and

$$\det(U) = \det\left(\begin{bmatrix} u_{1,1} & u_{1,2} \\ u_{2,1} & u_{2,2} \end{bmatrix}\right) = u_{1,1} \cdot u_{2,2} - u_{1,2} \cdot u_{2,1}.$$

So

$$\det(C_J - \lambda I) = \det\left(\begin{bmatrix} 0 & 1 \\ \frac{1}{2} & 0 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}\right) = \det\left(\begin{bmatrix} -\lambda & 1 \\ \frac{1}{2} & -\lambda \end{bmatrix}\right) = \lambda^2 - \frac{1}{2},$$

and $\lambda_{1,2}^J = \pm\sqrt{\frac{1}{2}} \approx \pm 0.7071$. So $\rho(C) = 0.7071$ and $\rho(C) < 1$.

For C_{GS} we have

$$\det(C_J - \lambda I) = \det\left(\begin{bmatrix} -\lambda & 1 \\ 0 & \frac{1}{2} - \lambda \end{bmatrix}\right) = \lambda\left(\frac{1}{2} - \lambda\right),$$

and $\lambda_1^{GS} = 0$ and $\lambda_2^{GS} = \frac{1}{2}$ and $\rho(C_{GS}) = \frac{1}{2}$.

The reason why Gauss-Seidel converges faster than Jacobi is that $\rho(C_{GS}) \leq \rho(C_J)$.

17 Krylov subspace methods

Given x^0 an initial guess for the solution x of the linear system $Ax = b$, A $n \times n$, consider the residual vector

$$r^0 := b - Ax^0.$$

The Krylov subspace generated by A and r^0 is the subspace of $\mathbf{R}^n$ defined by

$$\mathcal{K}^m(A, r^0) := \text{span}\{r^0, Ar^0, \dots A^{m-1}r^0\}.$$

This subspace has dimension less than or equal to m.

A **Krylov subspace method** is as method where the m-th approximation is such that

$$x^m = x^0 + v, \quad v \in \mathcal{K}^m(A, r^0)$$

and the residual $r^m := b - Ax^m$ satisfies

$$r^m \perp w, \quad \forall w \in \mathcal{L}^m,$$

where $\mathcal{L}^m$ is a subspace of $\mathbf{R}^n$ of dimension less than or equal to m.

Typical choices for $\mathcal{L}^m$ are:

$$\mathcal{L}^m = \begin{cases} \mathcal{K}^m(A, r^0) \\ \\ A\mathcal{K}^m(A, r^0) \end{cases}$$

The first choice leads to the so called Full Orthogonalization Method (FOM). When A is symmetric and positive definite, this method is equivalent to the famous Conjugate Gradient method (CG) . The second choice gives rise to the so called Generalized Minimal Residual method (GMRES). For more details on the implementation of these iterative techniques please refer to numerical linear algebra courses.

18 Preconditioning

Given

$$Ax = b$$

we want to find $M \approx A$ and M easy to "invert", such that

$$M^{-1}Ax = M^{-1}b$$

is "easier" to solve with an iterative method, i.e. the iterative methods converge faster. This is typically achieved if the choice of M leads to

$$\mathcal{K}(M^{-1}A) \leq \mathcal{K}(A),$$

where $\mathcal{K}(A)$ denotes the condition number of A.

To get a satisfactory preconditioner we need:

- $M \approx A$ must be such that linear systems of the type

$$Mz = w$$

  are easy to solve;

- $M \approx A$ must be a good approximation of A such that the product $M^{-1}A$ is close to the identity matrix, this implies that $\mathcal{K}(M^{-1}A)$ is small compared to $\mathcal{K}(A)$.

If one sapiently constructs M following the above guidelines, the iteration will converge significantly faster to the solution of the linear system. In the implementation one should carefully handle the extra operations involved in applying a Krylov subspace method to the preconditioned system instead of to the original system, in order not to loose all the computational gain given by using a preconditioner.