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Numerical Analysis

Lectures Notes

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Abstract

This document contains my notes on the course of Numerical Analysis held by Prof. Luca Heltai and Prof. Gianluigi Rozza for the Master Degree in Data Science and Scientific Computing at SISSA in the year 2020/2021. As they are a work in progress, every correction and suggestion is welcomed. Please, write me at: marco.sciorilli@gmail.com. A special thanks to Gabriele Sarti, as the basis for this work comes from its own notes on the same course.

Contents

Chapter 1

Rounding/truncation error, conditional error

1.1 Floating-point representation

Real number representation in $\mathbb{F}$ (the set of the floating-point numbers):

$$x = (-1)^s \cdot (0.a_1 a_2 ... a_t) \cdot \beta^e = (-1)^s \cdot m \cdot \beta^{e-t} \quad with\ a \neq 0 \tag{1.1}$$

- s is a sign bit (1 or 0)
- β is the basis adopted by computer (usually it is 2)
- m is the mantissa of length t made by digits a, with $0 \leq a_i \leq \beta - 1$
- e is the exponent

The set of number representable by a machine is characterized by β, t and the range (L, U) of the exponent. It is commonly denoted as $\mathbb{F}(\beta, t, L, U)$.
The roundoff error occur when we replace $x \neq 0$ with its $\mathbb{F}$ representation, $\hat{x}$, and is defined as

$$\frac{|x - \hat{x}|}{|x|} \leq \frac{1}{2}\epsilon_M \quad with\ \epsilon_M = \beta^{1-t} \tag{1.2}$$

Where ϵ_M is the machine epsilon: the minimal variation representable by a machine

$$\epsilon_M \text{ the largest number } | \quad fl(1 + \epsilon_M) = fl(1) \tag{1.3}$$

Where $fl()$ is the floating-point representation of a number. $\frac{1}{2}\epsilon_M$ is the roundoff unit, $|x - \hat{x}|$ is the absolute error, and $\frac{|x-\hat{x}|}{|x|}$ is the relative error of the approximation operated. The relative error accounts for the order of magnitude of x.
0 is not part of $\mathbb{F}$ and is therefore handled separately. A number exceeding the lower bound is treated as 0 while numbers exceeding the upper bound is treated as inf. $\mathbb{F}$ is not homogeneously dense, but it is denser near 0, and less dense near infinity.
In $\mathbb{F}$ associativity and distributivity are not always respected, as for the case of the loss of significant digits. Indeterminate forms as $\frac{0}{0}$ and $\frac{inf}{inf}$ produces error flagged as NaN.

1.2 Complex numbers

The classic representation of complex number is

$$z = x + iy = \varphi e^{i\theta} = \varphi(cos\theta + isen\theta) \tag{1.4}$$

Where $i = \sqrt{-1}$, $x = Re(z)$, $y(Im)$ and $\varphi = \sqrt{x^2 + y^2}$.
z is a complex number ($\in \mathbb{C}$ with a real part x and an imaginary part y, both represented by two floating-point numbers. Its modulus is φ, and its complex conjugate is

$$\overline{z} = x - iy = \varphi e^{-i\theta} = \varphi(cos\theta - isen\theta) \tag{1.5}$$

The complex conjugate is used in the conjugate transposition of matrices

$$(A_{ij})^* = \overline{A_{ij}} \tag{1.6}$$

1.3 Matrices

Some properties of matrices are

- $A + B = (a_{ij}) + (b_{ij}) = (a_{ij} + b_{ij})$
- $\lambda A = (\lambda a_{ij})$
- $C_{m\times n} = A_{m\times p} B_{p\times n} = (c_{ij}) = \sum_{k=1}^{p} a_{ik} b_{kj}$

If a matrix is diagonal, its determinant is the product of diagonal elements. A matrix is lower/upper triangular if all the elements above/under the main diagonal are zero.
If $A \in \mathbb{R}^{m\times n}$ and its transpose $A^t \in \mathbb{R}^{n\times m}$, A is symmetrical if $A = A^t$. If $A = A^H = \overline{A}^t$, A is hermitian.

1.4 Vectors

A set of vectors $y_1, ..., y_m$ is linearly independent if

$$a_1 y_1 + ... + a_m y_m = 0 \Leftrightarrow a_1, ..., a_m = 0 \tag{1.7}$$

B is a basis for $\mathbb{R}^n$ or $\mathbb{C}^n$ if $B = y_1, ..., y_n$ and $y_1, ..., y_n$ are all independent vectors. Any vector w in $\mathbb{R}^n$ can then be written as

$$w = \sum_{k=1}^{n} a_k y_k \tag{1.8}$$

a_k are unique components of w in relation to B.
THe scalar dot product of v and w is defined as

$$(v, w) = w^t v = \sum_{k=1}^{n} a_k b_k \tag{1.9}$$

with a and b respectively components of v and w.
The modulus of a vector v is given by the euclidean norm formula

$$\|v\| = \sqrt{(v,v)} = \sqrt{\sum_{k=1}^{n} v_k^2} \tag{1.10}$$

The vector product (cross product) of $v, w \in \mathbb{R}^3$ is the vector u orthogonal to v and w, with modulus $|u| = |v||w|sin\alpha$.
$v \in \mathbb{C}^n$ is an eigenvector of $A \in \mathbb{C}^{n\times m}$ associated with eigenvalue λ if

$$Av = \lambda v \tag{1.11}$$

The eigenvalues of diagonal and triangular matrices are the elements on the diagonal.
A matrix is said to be positive definite if

$$z^t Az \geq 0 \ \forall \ z \in \mathbb{R}^n \tag{1.12}$$

1.5 Real Functions

If $f(\alpha) = 0$, α is a zero r root of f. It is called simple if $f'(\alpha) \neq 0$, multiple otherwise.
The space $\mathbb{P}_n$ of polynomials of degree $\leq n$ is defined as

$$p_n(x) = \sum_{k=0}^{n} a_k x^k \tag{1.13}$$

with a_k given coefficients.
The number of zeros cannot usually be estimated a priori (except for polynomials, where its $= n$). The value for p_n zeros cannot be computed with an explicit formula for $n \geq 5$.
Foundamental theorem of integration, for f continuous in $[a, b]$

$$F(x) = \int_a^x f(x)dt \ \forall x \in [a,b) \ \Rightarrow \ F'(x) = f(x) \ \forall \ x \in [a,b) \tag{1.14}$$

First mean-value theorem for integrals, for f continuous in $[a, b)$ and $x_1, x_2 \in [a, b)$ with $x_1 < x_2$

$$\exists \xi \in (x_1, x_2) \ s.t. \ f(\xi) = \frac{1}{x_2 - x_1} \int_{x_1}^{x_2} f(t)dt \tag{1.15}$$

$f \in [a, b]$ is differentiable in $x \in (a, b)$ if

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h} \tag{1.16}$$

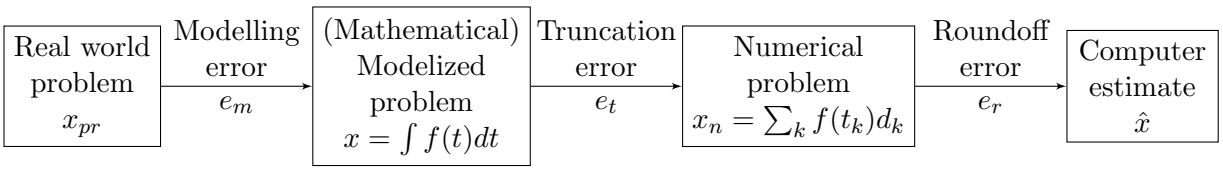
exist and is finite.
Mean value theorem: if $f \in C^\circ([a, b])$ and is differentiable in (a, b)

$$\exists \xi \in (a,b) \ s.t. \ f'(\xi) = \frac{f(b) - f(a)}{b - a} \tag{1.17}$$

Taylor expansion of p_n: if $f \in C^\circ([x_0 - c, x_0 + c])$ (a neighbovarphiod of x_0), f can be approximated in that interval as

$$T_n(x) = f(x_0) + (x - x_0)f'(x_0) + ... + \frac{1}{n!}(x - x_0)^n f^{(n)}(x_0) = \sum_{k=0}^{n} \frac{(x - x_0)^k}{K!} f^{(k)}(x_0) \tag{1.18}$$

1.6 Estimating errors



The sum of truncation error derived from reducing a problem to a finite set of operations and roundoff error coming from a machine representation is called computational error e_c

$$e_c^{abs} = |x - \hat{x}| \quad e_c^{rel} = \frac{|x - \hat{x}|}{|x|} \tag{1.19}$$

To convert a mathematical problem in numerical form we use discretization parameter h, positive.
if $(num) \to (mat)$ as $h \to 0$ the numericl process is said to be convergent.
If we can bound e_c as $e_c \leq Ch^p$ we say that the method is convergent of order p. if a lower bound $C'h^p \leq e_c$ also exists, we can approximate the final error.
Logarithmic scale is effective for numerical methods since lines slopes represent the order of convergence for each method. The semi-logarithmic scale is also used to visualize functions that span many orders of magnitude in y in a short x interval.
The computational cost is O (ops, operations) and can be constant, linear, polynomial, exponential, factorial, ecc.
Numerical approximation can be performed exclusively on well-posed problems, thats to say problems for which the solution:

- Exists
- Is unique
- Depends continuously on data

The total error is:

$$f(x) - \hat{f}(\hat{x}) = \underbrace{\hat{f}(\hat{x}) - f(\hat{x})}_{\substack{\text{computation} \\ \text{error} \\ (e_c = e_t + e_r)}} + \underbrace{f(\hat{x}) - f(x)}_{\substack{\text{propagated data} \\ \text{error} \\ \text{(independent from f)}}} \tag{1.20}$$

ex. finite differences approximation ($f'(x) = \lim_{h\to 0} \frac{f(x-h)-f(x)}{h}$)

- Truncation error (obtained through Taylors) $\sim \frac{1}{2}|(f''(x)|h + O(h^2)$
- Rounding error $\sim \frac{2\epsilon}{h}$ with ϵ =machine precision

The optimal h is therefore $h = 2\sqrt{\frac{\epsilon}{|f''(x)|}}$

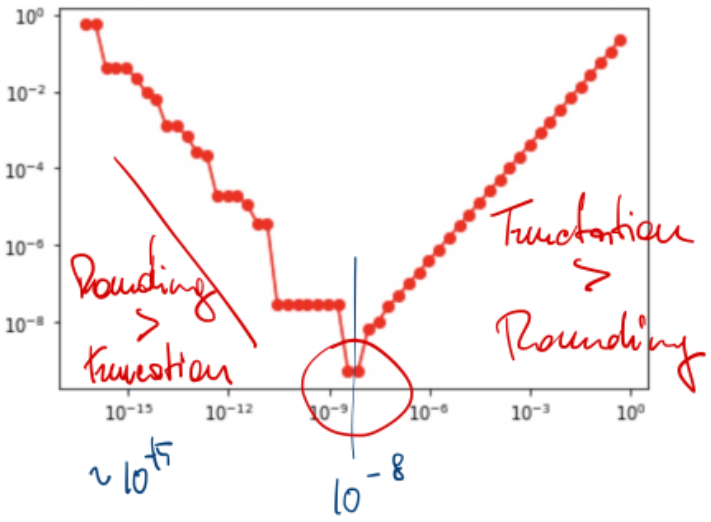


Figure 1.1: Plot of total error vs h. The optimal value of h which minimize the total error is reached when $h \sim \sqrt{\epsilon}$

Problem stability: small changes in input data produce small variation on the output. It is a synonymous of well-posedness.
Given δ a perturbation in data s.t. $d + \delta d \in D$, and $x + \delta x$ the perturbed solution, then

$$\forall d \in D \ \exists \eta(d) \text{ and } K \ s.t. \ \|\delta d\|_d < \eta \in D \Rightarrow \|\delta x\|_x < K\|\delta d\|_d \tag{1.21}$$

Condition numbers: it can be either relative or absolute and measure problem sensitiveness with regards to input data.
If we define $\Delta y = f(x) - f(\hat{x})$ and $\Delta x = x - \hat{x}$, we have that the relative condition numbers is

$$K_{rel} = \frac{\frac{\Delta y}{y}}{\frac{\Delta x}{x}} \approx |f'(x)| \frac{|x|}{|f(x)|} \tag{1.22}$$

And the absolute condition number is:

$$K_{abs} = \frac{\Delta y}{\Delta x} \quad (\text{if } f(x) \text{ or } x = 0\ ) \approx |f'(x)| \tag{1.23}$$

If $K \gg 1$ the problem is ill-posed (sensitive, unstable) and is thus not approximable through numerical methods.
A numerical approximation can be seen as a sequence of simpler approximating problems that converge to the original one

$$\lim_{n\to\infty} \|y_n - y\| = \lim_{n\to\infty} \|x_n - x\| = 0 \text{ is as } \lim_{n\to\infty} f_n(x) = f(x) \tag{1.24}$$

1.7 Banach Spaces

Given $\vec{v}$ over $\mathbb{R}$ or $\mathbb{C}$, a seminorm is a function $|\cdot| : V \to \mathbb{C}$ which satisfy:

- $|cf| = |c||f|\ \forall c \in \mathbb{C}$ (homogeneity)
- $|f+g| \leq |f| + |g|$ (triangular inequality)

$\vec{v}$ is a vector space and the norm is a linear mapping.
If $|f| = 0$ iff $f = 0$ (positive definite) is also verified, we have a norm. A vector space is said to be complete if every Cauchy sequence in that space converges to one of the space's elements.
A complete vector space with a norm is called Banach Space.
The scalar product is a mapping $V \times V \to \mathbb{C}$ which is:

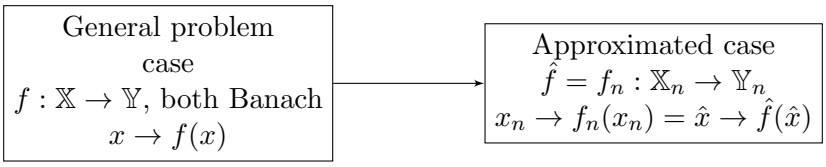
- Linear: $(\alpha_1 v_1 + \alpha_2 v_2, w) = \alpha_1(v_1, w) + \alpha_2(v_2, w)$
- Symmetric:$(v, w) = (\overline{w, v})$
- Positive definite: $(v_1, v_2) \geq 0 \ \ \forall v_1, v_2$ and $(v_1, v_2) = 0$ iff $v_1, v_2 = 0$

A Banach space with scalar product and a norm $\|f\| = (f, f)$ induced by the product is called Hilbert space.
Examples of norms in the Banach spaces:

- $\|x\|_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$
- $\|x\|_1 = \sum_{i=1}^n |x_i|$
- $\|x\|_2 = \sqrt{x_1^2 + x_2^2}$ (euclidean norm)
- $\|x\|_\infty = \sup_{1 \leq i \leq n}(x_i)$

In a finite-dimensional vector space (dimension is given by the number of vectors in the basis), all norms are equivalents:

$$\forall \|\cdot\|_a, \|\cdot\|_b \ \exists 0 \leq c_1 \leq c_2 \ s.t. \ c_1\|x\|_b \leq \|x\|_a \leq c_2\|x\|_b \tag{1.25}$$



1.8 Converge, consistency and Lax-Richtmyer

A numerical method is convergent if the approximation $\hat{f}_n$ of a problem f satisfies:

- $\lim_{n\to\infty} \|x_n - x\|_{\mathbb{X}} = 0$
- $\lim_{n\to\infty} \left\| \hat{f}_n(\underbrace{x_n}_{\text{approx.}}) - f(x) \right\|_{\mathbb{X}} = 0$

A numerical problem is consistent when, if $x \in \mathbb{X}_n \forall n$, we have that

$$\lim_{n\to\infty} \left\| f_n(\underbrace{x}_{\text{exact}}) - f(x) \right\| = 0 \tag{1.26}$$

Example 1. *Sum of two numbers*

- $\mathbb{X} : \mathbb{R}^2, \|x\|_{\mathbb{X}} = |x_1| + |x_2| = \|x\|_{l^1(\mathbb{R}^2)}$
- $\mathbb{R}, \|y\|_{\mathbb{Y}} = |y| = \|y\|_{l^1(\mathbb{R}^1}$

$$K_{rel} = \frac{|\Delta y|}{|\Delta x|} \cdot \frac{|x|}{|y|} \Rightarrow K_{rel} \leq \frac{|x_1| + |x_2|}{|x_1 + x_2|} \tag{1.27}$$

Result: *Unstable in* $\mathbb{F}$ *when* $x_1 \cong -x_2 \Rightarrow K_{rel} \to \infty$

- A convergent approximation is always stable.
- Finite differences are unstable since they are a sum of two numbers with close absolute value and opposite sign.
- For integration, $K_{\text{rel}} = \frac{\int |x|}{|\int x|}$, so it is ill-posed when $x \sim 0$.
- The condition number of a matrix A is $K_{\text{rel}} = \left\|A^{-1}\right\| \|A\|$
  This usually corresponds to

$$K(A) = \frac{\left|\lambda_{\text{MAX}(A)}\right|}{|\lambda_{\text{MAX}}(A)|} \tag{1.28}$$

The **Lax-Richtmyer theorem** says that if a problem is consistent, then stability and convergence are equivalent.

- Stability controls perturbation in data and their impact.
- Consistency controls bad approximation of a problem.
- Convergence controls bad discretizations of the problem space (and includes stability).

A method is consistent if the residual (error produced by plugging the exact solution in the scheme) goes to 0 as $h \to 0$

Chapter 2

Nonlinear equation

We may want to find the roots of the non linear functions ($\alpha \in \mathbb{R}$ *s.t.* $f(\alpha) = 0$) in a computational way. Most common approaches are iterative, sinche there is no explicit solving formula for $p \in \mathbb{R}^n$, with $n \geq 5$ (**Abel's theorem**).

2.1 Bisection method (linear convergence)

It is used to compute the root of a function f on interval $[a, b]$.
Constrains for convergence:

- f should be continuous on $[a, b]$.
- Interval end points should have different sign ($f(a)f(b) < 0$) to have at least 1 solution (**theorem of zeros for continuous functions**)

We generate a sequence of intervals whose length is halved at each step, with $x^{(k)}$ being the midpoint at step k.
The error of estimation at step k is:

$$\left|e^{(k)}\right| = \left|x^{(k)} - \alpha\right| < \frac{1}{2}\left|I^{(k)}\right| = \left(\frac{1}{2}\right)^{k+1}(b-a) \tag{2.1}$$

In order to ensure that the error $\left|e^{(k)} < \epsilon\right|$, we carry out K_{mm} iterations at least:

$$K_{mm} > \log_2\left(\frac{b-a}{\epsilon}\right) - 1 \tag{2.2}$$

The error does not decrease monotonically. The only possible stopping criterion is controlling the size of $I^{(k)}$.

2.2 Newton's method (Quadratic or linear convergence)

H is used to compute the root of a function f by using the values of f and f' (more efficient than bisection).
Constrains for convergence:

- $f : \mathbb{R} \to \mathbb{R}$ should be differentiable.
- x_0 is sufficiently close to α given f (estimate through graph and bisection).

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})^2},\ k = 0, 1, ... \tag{2.3}$$

If $f \in \mathcal{C}^2$, we have that $\lim_{k\to\infty} \frac{x^{(k+1)}}{(x^{(k)}-\alpha)^2} = \frac{f''(\alpha)}{2f'(\alpha)}$ than we have quadratic convergence.
If f has zeros with multiplicity $m > 1$, if $f'(x) \neq 0\ \forall x \in I(\alpha)$, the method converges linearly. To restore quadratic convergence, one can use the **modified Newton method**, or **adaptive Newton methods** if m is unknown.

$$x^{(k+1)} = x^{(k)} - m\frac{f(x^(k))}{f'(x^{(k)})}, \quad k = 0, 1, ... \tag{2.4}$$

(α of f has multiplicity m iff $f(\alpha) = ... = f^{(m-1)}(\alpha) = 0$ and $f^{(m)}(\alpha) \neq 0$).
Stopping criterion: Control of the movement

$$\left|x^{(k+1)} - x^{(k)}\right| < \epsilon \tag{2.5}$$

We can also perform a test on the residual which is valid only if $|f'(x)| \simeq 1\ \forall x \in I(\alpha)$, else it produces an over or underestimation of error

$$\left|r^{(k_{\min})}\right| = \left|f(x^{(k_{\min})})\right| < \epsilon \tag{2.6}$$

2.3 Secant method (sublinear convergence)

In case $f'(x)$ is not available, we can replace its value with an incremental ration based on previous values

$$x^{(k+1)} = x^{(k)} - \Big(\frac{f(x^{(k)}) - f(x^{k-1})}{x^{(k)} - x^{(k-1)}}\Big)^{-1} f(x^{(k)}) \tag{2.7}$$

Constrains for convergence:

- α has $m = 1$ (for superlinear).
- $x^{(0)}$ is selected in $I(\alpha)$ suitable.
- $f'(x) \neq 0\ \forall x \in I(\alpha)$

If $m = 1$ and $f \in \mathcal{C}^2(I(\alpha))$, $\exists c > 0$ s.t.

$$\left|x^{(k+1)} - \alpha\right| \leq c\left|x^{(k)} - \alpha\right|^P \quad \text{with } p \approx 1.618 \tag{2.8}$$

Else the method converges linearly.

2.4 Systems of nonlinear equations

Given $f_1, ..., f_n$ nonlinear functions in $x_1, ..., x_n$, we can set $f = (f_1, ..., f_n)^T$ and $\overline{x} = (x_1, ..., x_n)^T$ to write a system

$$\overline{f}(\overline{x}) = 0 \tag{2.9}$$

We can extend the Newton method to that system by replacing the f' with the Jacobian Matrix $J_{\overline{f}}$, as

$$(J_{\overline{f}})_{ij} = \frac{\partial f_i}{\partial x_j} \quad i, j = 1, ..., n \tag{2.10}$$

The secant method can also be adopted by recursively defining matrices B_k which are suitable approximation of $J_{\overline{f}}(x^0)$ (**Broyden Method**). This belongs to the family of quasi-newton methods.

2.5 Fixed point iterations

Given a function $\phi : [a, b] \to \mathbb{R}$, we want to find an α so that

$$\phi(\alpha) = \alpha \tag{2.11}$$

If α exists, it is called a **fixed point** of ϕ and it could be computed as follows:

$$x^{(k+1)} = \phi(x^{(k)}),\ k \geq 0 \quad \text{with } x^{(0)} \text{ initial guess} \tag{2.12}$$

ϕ is called the iteration function. The Newton method is a special case of fixed point iteration where

$$\phi_N(x) = x - \frac{f(x)}{f'(x)} \tag{2.13}$$

2.6 Global convergence

1. Iff $\phi(x)$ is continuous in $[a, b]$ and $\phi(x) \in [a, b]$ $\forall x \in [a, b]$ then there exists at least one $\alpha \in [a, b]$.
2. Moreover, if $\exists L < 1$ (**Asymptotic convergence factor**) s.t.

$$|\phi(x_1) - \phi(x_2)| \leq L|x_1 - x_2| \ \forall x_1, x_2 \in [a, b] \tag{2.14}$$

   then $\alpha \in [a, b]$ is unique and the iteration converges to α $\forall x^{(0)} \in [a, b]$

Proof. 1. Form our assumptions we have that $g(x) = \phi(x) - x$ is continuous in $[a, b]$, with:

$$g(a) = \phi(a) - a \geq 0 \quad \text{and} \quad g(b) = \phi(b) - b \leq 0 \tag{2.15}$$

For theorem of zeroes for c functions, we know that g has at least 1 zeros, and thus $\exists \alpha$ for ϕ in $[a, b]$.

2. If two fixed points existed, we would have

$$|\alpha_1 - \alpha_2| = |\phi(\alpha_1) - \phi(\alpha_2)| \leq L|\alpha_1 - \alpha_2| < |\alpha_1 - \alpha_2| \tag{2.16}$$

which is absurd for $L < 1$. For x^0 in $[a, b]$ and $x^{(k+1)} = \phi(x^{(k)})$, we have

$$0 \leq \left|x^{(k+1)} - \alpha\right| = \left|\phi(x^{(k)}) - \phi(\alpha)\right| \leq L\left|x^{(k)} - \alpha\right| \Rightarrow \frac{\left|x^{(k)} - \alpha\right|}{x^{(0)} - \alpha} \leq L^k \tag{2.17}$$

The smaller the L, the faster the convergence.
Since $L < 1$, for $k \to \infty$, we notice

$$\lim_{k\to\infty} \left|x^{(k)} - \alpha\right| \leq \lim_{k\to\infty} L^k = 0 \tag{2.18}$$

Which is convergence.

□

2.7 Local convergence (Ostrowski's theorem)

If ϕ is a continuous and differentiable function on $[a, b]$, with fixed point α, and $|\phi'(\alpha)| < 1$ then $\exists\delta > 0$ s.t.

$$\left|x^{(0)} - \alpha\right| \leq \delta \quad \forall x^{(0)} \text{ in } [a, b] \tag{2.19}$$

for which the $x^{(k)}$ converges to α. It holds

$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{x^{(k)} - \alpha} = \phi'(\alpha) \tag{2.20}$$

$\forall c$ s.t. $0 < |\phi'(\alpha)| < c < 1$, for large k: $\left|x^{(k+1)} - \alpha\right| \leq c\left|x^{(k)} - \alpha\right|$
If $|\phi'(\alpha) > 1|$, the method diverges. If $|\phi'(\alpha)| = 1$, it depends on the function.

2.8 Quadratic convergence

If $\phi \in C^2([a, b])$ and α is fixed point of ϕ, with ϕ having local convergence. Then, if $\phi'(\alpha) = 0$ and $\phi''(\alpha) \neq 0$, fixed point converges with order 2 and

$$\lim_{k\to\infty} \frac{x^{(k+1)} - \alpha}{(x^{(k)} - \alpha)^2} = \frac{1}{2}\phi''(\alpha) \tag{2.21}$$

2.9 Stopping criteria

Error estimator at step k is

$$\alpha - x^{(k)} = e^{(k)} \approx \frac{1}{(1 - \phi'(\alpha))}(x^{(k+1)} - x^{(k)}) \tag{2.22}$$

Satisfactory when we have quadratic convergence (since $\phi'(\alpha) = 0$) or when $-1 < \phi'(\alpha) < 0$, problems when $\phi'(\alpha) \simeq 1$.
In that case we can use the central of the residual as described for newton method.

2.10 Aitken method

If ϕ converges linearly to α, there must be a X s.t. $\phi(x^{(k)}) - \alpha = X(x^{(k)} - \alpha)$. This allows us to obtain a better estimate of $x^{(k+1)}$ than $\phi(x^{(k)})$ (the **Aktken's extrapolation formula, Stefferson's method**)

$$\alpha = x^{(k)} + \frac{(\phi(x^{(k)} - x^{(k)})}{(1-\lambda)} \quad \text{with}$$
$$\lambda^{(k)} = \frac{\phi(\phi(x^{(k)})) - \phi(x^{(k)})}{\phi(x^{(k)}) - x^{(k)}} \quad \text{given}$$
$$\lim_{k\to\infty} \lambda^{(k)} = \phi'(\alpha)$$
$$\Rightarrow x^{(k+1)} = x^{(k)} - \frac{(\phi(x^{(k)}) - x^{(k)})^2}{\phi(\phi(x^{(k)})) - 2\phi(x^{(k)}) + x^{(k)}} \quad k \geq 0$$

The derived function $\phi_\Delta(x)$ has the same α as $\phi(x)$, but converges faster:

- Linear $\phi \to$ Quadratic ϕ_Δ
- $p \geq 2$ $\phi \to 2p - 1$ ϕ_Δ
- Linearly with $m \geq 2$ $\phi \to$ Linearly with $L = 1 - \frac{1}{m}\phi_\Delta$

H may converge even if normal FPI diverges.

2.11 Rope method

Obtained by modifying the Newton method, replacing $f'(x)$ with a fixed q

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)}}{q} \quad k = 0, 1, ... \tag{2.23}$$

e.g. $q = \frac{f(b)-f(a)}{b-a}$ in $[a, b]$.
Since it is a FPI with $\phi(x) = x - \frac{1}{q}f(x)$, we have convergence when

$$\phi'(x) = \left|1 - \frac{1}{q}f'(\alpha)\right| < 1 \tag{2.24}$$

Chapter 3

Interpolation

3.1 Approximation

Approximating a set of data or a function in $[a, b]$ consists in finding a suitable function $\tilde{f}$ that represents them with enough accuracy.
We can use Taylor polynomials to approximate complex functions but require many computations and have unpredictable behaviors on the sides of the domain.
If X is a Banach space and $M \subseteq X$, $\tilde{f} \in M$ is the best approximation of a function $f \in X$ when

$$\left\| f - \tilde{f} \right\| = E(f) = \inf_{\tilde{f} \in M} \left\| f - \tilde{f} \right\| \tag{3.1}$$

- $\tilde{f} \in M$ is the best approximation of the f in M.
- If M is a finite-dimensional subspace of X, then $\exists\ \tilde{f}$ B.A. of f in M (existence theorem).
- If X is strictly convex (any x, y on the unit sphere ∂B are joined by a segment that touches ∂B only in x, y), than $\tilde{f}$ is unique (uniqueness theorem).

3.2 Interpolation

Given $n + 1$ points $\{q_i = (x_i, y_i)\}_{i=0}^{n}$ on an interval, we want to find the function φ s.t. $\varphi(x_i) = y_i \forall i$.
We call this function φ **interpolant**, and the point nodes. We say that φ interpolates y_i in nodes q_i.
Interpolation is a form of approximation that could be used both to simplify a complex function in order to make it easier to derive or to understand data distributions. The iterpolants can be polynomial, trigonometric, rational, ecc.

3.3 Lagrange interpolation (φ is polynomial)

Given $n+1$ couples $\{x_i, y_i\}$, $i = 0, ..., n$ with x_i as nodes, we want to find a polynomial of degree $\leq n$ ($\pi_n \in \mathbb{P}^n$) s.t.

$$\pi_n(x_i) = y_i \quad \forall i \tag{3.2}$$

If y_i represent the values of a continuous f, π_n is the interpolant of f, denoted $\pi_n f$
In this setting $\exists!\ \pi_n \in \mathbb{P}^n$ s.t. $\pi_n(x_i) = y_i\ \forall i$
In order to obtain an expression for π_n, we study a special case in which $y_i = 0\ \forall j$ except when $y_{j=k} = 1$.

$$p_k \in \mathbb{P}_n, \quad p_k(x_j) = \underbrace{\delta_{jk}}_{\text{Kronecker symbol}} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{otherwise} \end{cases} \tag{3.3}$$

φ_k is called **Lagrange basis** since it is a basis for $\mathbb{P}^n$. It has the following expression (also called Lagrange characteristic polynomials)

$$\varphi_k(x) = \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{x - x_j}{x_k - x_j} \tag{3.4}$$

We define the Lagrange interpolant of f on nodes $x_0, ..., x_n$ the following linear combination of degree n

$$\mathcal{L}^n f = \sum_{k=0}^{n} f(x_k)\varphi_k(x) \tag{3.5}$$

The Lagrange basis is especially fit for good approximation since other polynomial sets may be ill-conditioned for the approximation task.
The example P^n generate the **Vandermonde matrix**, which is ill conditioned since for n large, rightmost columns will be very similar, making the matrix hardly invertible

$$B = (B_{ij}) = \begin{bmatrix} 1 & q_0 & q_0^2 & ... & q_0^n \\ 1 & q_1 & q_1^2 & ... & q_1^n \\ ... & ... & ... & ... & ... \\ 1 & q_n & q_n^2 & ... & q_n^n \end{bmatrix} = (q_i^s) \tag{3.6}$$

3.4 Interpolation error

$\{x_i,\ i = 0, ..., n\}$ are $(n+1)$ nodes on a bounded interval I. Given $f \in C^{n+1}(I)$. Then, $\forall x \in I \quad \exists \xi_x \in I$ s.t.

$$E_n f(x) = f(x) - \mathcal{L}^n f(x) = \frac{f^{(n+1)}(\xi_x) w(x)}{(n+1)!}, \quad \text{with } w(x) \prod_{i=0}^{n} x - x_i \tag{3.7}$$

Since $\|\cdot\|_\infty$ represent the highest value (sup) of a function, we can bound the error as

$$\|f(x) - \mathcal{L}^n f(x)\|_\infty \leq \frac{\left\|f^{(n+1)}(\xi)\right\|_\infty \|w(x)\|_\infty}{(n+1)!} \tag{3.8}$$

If f is analytically extendable in an oval $O(a,b,R)$ with $R>0$

$$\Rightarrow \left\| f^{(n+1)} \right\|_{\infty,\overline{O(a,b,R)}} \leq \frac{(n+1)!}{R^{n+1}} \|f\|_{\infty,\overline{O(a,b,R)}} \tag{3.9}$$

Thus, we can control the $(n+1)$ derivative directly with f.
Also

$$\|f - \mathcal{L}^n f\|_{\infty,[a,b]} \leq \frac{(n+1)!}{R^{n+1}} \|f\|_{\infty,O(a,b,R)} \left(\frac{|b-a|}{R}\right)^{n+1} \tag{3.10}$$

Then increasing the degree n of the interpolator does not guarantee a better approximation of n. Indeed, we may have that

$$\lim_{n\to\infty} \|f - \mathcal{L}^n f\|_\infty = \infty \tag{3.11}$$

3.5 Runge counterexample

$f(x) = \frac{1}{(1+x^2)}$ is interpolated at equispaced nodes in $I=[-s,s]$. The error$\|f - \mathcal{L}^n f\|_\infty$ tends to infinity when $n \to \infty$.
The presence of severe oscillations of $\mathcal{L}f$ w.r.t. f, especially near the endpoints, indicates lack of convergence. This is also called **Runge's phenomenon**.

3.6 Stability of interpolation

We want to estimate the impact of perturbed values $\hat{f}(x)$ on the interpolator $\mathcal{L}^n f$. We have that

$$\left\| \mathcal{L}^n f - \mathcal{L}^n \hat{f} \right\|_\infty = \Lambda_n(\{x_i\}_{i=0}^n) \left\| f - \hat{f} \right\| \tag{3.12}$$

where

$$\Lambda_n(\{x_i\}_{i=0}^n) = \|\sigma_{i=0}^n |\varphi_i(x)|\|_\infty \tag{3.13}$$

is the **Labesgue's constant** depending on interpolation nodes.
From the fisrt formula, we have that small variations in f yield small changes in $\mathcal{L}^n f$ if Λ is small. Therefore, Λ can be regarded as a condition number for interpolation.
It can be proved that $\|\mathcal{L}^n f\| \leq \Lambda_n(x)$.
For Lagrange interpolation at equispaced nodes

$$\Lambda_n(x) \simeq \frac{2^{n+1}}{e \cdot n(\log n + \gamma)}, \quad \text{with } e \approx 2.718 \text{ and } \gamma \approx 0.547 \tag{3.14}$$

For large values of n, this becomes unstable.

3.7 Distance from B.A.

If $p = \inf_{x \in \mathbb{P}^n} \|f - x\|_\infty$ with $\{x_i\}_{i=0}^n$ $(n+1)$ nodes, then

$$\begin{aligned}\|f - \mathcal{L}^n f\| =& \|f - p - \mathcal{L}^n(f-p)\| \\ \leq& \|f-p\|_\infty + \|\mathcal{L}^n(f-p)\|_\infty \\ \leq& \|I - \mathcal{L}^n\|_{\mathcal{L}} \|f-p\|_\infty \\ \leq& (\|I\|_{\mathcal{L}} - \|\mathcal{L}^n\|_{\mathcal{L}}) \|f-p\|_\infty \\ \leq& (1 + \|\mathcal{L}^n\|_{\mathcal{L}}) \|f-p\|_\infty\end{aligned}$$

where I is an operator for $f - p$ and $\|\mathcal{L}^n\|_{\mathcal{L}} = \sup_{n \neq 0} \frac{\|\mathcal{L}^n n\|_\infty}{\|n\|_\infty}$.
p is the best approximation of f on nodes $\{x_i\}_{i=0}^n$.

3.8 Chebyshev nodes

In order to minimize Λ and thus avoid Runge's phenomenon, we can use Chebyshev nodes on interval $[a, b]$ defined as

$$x_i = \frac{a+b}{2} + \frac{b-a}{2} \hat{x}_i \tag{3.15}$$

where $\hat{x}_i = -\cos\left(\frac{\pi i}{n}\right),\ i = 0, ..., n$.
The nodes are equispaced on the semicirconference of diameter $[a, b]$ and are clustered towards the endpoints of the interval.
For Chebyshev nodes if f is continuously differentiabe in $[a, b]$, $\mathcal{L}^n f$ converges to f as $n \to \infty$ $\forall x \in [a, b]$

3.9 Erdos theorem

$\forall X$, where X is an infinite triangular matrix of interpolation points

$$X = \begin{bmatrix} 0 & 0 & 0 & ... & 0 \\ x_0 & 0 & 0 & ... & 0 \\ x_0 & x_1 & 0 & ... & 0 \\ ... & ... & ... & ... & ... \\ x_0 & x_1 & x_2 & ... & x_n \end{bmatrix} \tag{3.16}$$

we have

$$\Lambda_n(X) \geq \frac{2}{\pi} \log(n+1) - c \tag{3.17}$$

For Chebyshev nodes we have $\Lambda_n(X) \leq \frac{2}{\pi \log(n+1)+1}$.
For equispaced nodes we have $\Lambda_n(X) \leq \frac{2^{n+1}}{c(n \log n)}$.

3.10 Faber theorem

$$\forall x\ \exists f \in C^0([a, b])\ s.t. \|f - \mathcal{L}^n f\|_\infty \nrightarrow 0 \tag{3.18}$$

The Faber theorem proves that even on Chebyshev nodes not all continuous function will converge when used for interpolation.

3.11 Weierstrass approximation theorem

Suppose $f \in C^0([a,b])$. Then,

$$\forall \epsilon > 0 \ \exists p \in \mathbb{P}^n \ s.t. \ \|f - p\| < \epsilon, \ \forall x \in [a,b] \tag{3.19}$$

It shows that polynomial functions are dense in $C^0([a,b])$ and each polynomial can be uniformly approximated by one with rational coefficients.

3.12 Bernstein coefficients

The $n+1$ Bernstein basis for $\mathbb{P}^n$ are defined as

$$b_{n,i}(x) = \binom{n}{i} x^i (1-x)^{n-i}, \ i = 0, ..., n \tag{3.20}$$

$b_{n,i}$ is the $i-th$ polynomial in the Bernstein basis of degree n.
A linear combination of $b_{n,i}$ is called a Bernestein polynomial of degree n based on function f

$$B_n f(x) = \sum_{k=0}^{n} f(\frac{k}{n}) b_{n,k}(x) \tag{3.21}$$

$\forall x$ this is a weighted average of the $n+1$ values $f(\frac{k}{n})$ called bernstein coefficients.
Properties:

- $\sum_{i=0}^{n} b_{i,n} = (1 - x + x)^n = 1^n = 1 \quad \forall x \in [0,1]$
- $b_{i,n} \geq 0 \quad \forall x \in [0,1]$
- B_n is a linear positive operator: $B_n f \geq 0$ if $f \geq 0$
- $B_n f\left(\frac{i}{n}\right) \neq f\left(\frac{i}{n}\right)$ and if $f \in C^0([a,b])$ we have that $B_n f(x) \to f(x)$ as $n \to \infty$

The convergence is not pointwise as in interpolation, but uniform

$$\lim_{n \to \infty} \|f(x) - B_n f(x)\|_\infty = 0 \quad \text{with} \quad 0 \leq x \leq 1 \tag{3.22}$$

3.13 Qualitative proof of Weierstrass theorem

$\forall f \in C(I)$ and $\forall x_0 \in I$, we can find a quadratic function q s.t. $q > f \ \forall x$, but $q(x_0)$ is close to $f(x_0)$. The same can be done with $q < f$.

$$q = f(x) \pm \left(\frac{\epsilon}{2} + \frac{\|f\|_\infty}{2\sigma}(x - x_0)^2\right)$$

with

$$|x_1 - x_2| \leq \sigma \to |f(x_1) - f(x_2)| \leq \frac{\epsilon}{2}$$

$$q = ax^2 + bx + c$$

$$M = \max_{x_0 \in [a,b]} (a(x_0), b(x_0), c(x_0))$$

M depends exclusively on $\|f\|$, ϵ and σ but not on x_0.
By choosing a large n we have $\|f_i - B_n\| \leq \frac{\epsilon}{M}$. Using the triangle inequality we get $\|q - B_n q\| \leq 3\epsilon$. We have then

$$B_n f(x_0) \leq B_n q(x_0) \leq q(x_0) + 3\epsilon = f(x_0) + 4\epsilon \tag{3.23}$$

Same can be done below, having that

$$\forall x_0 \ f(x_0) - \epsilon \leq B_n f(x_0) \leq f(x_0) + \epsilon \tag{3.24}$$

So

$$\rightarrow \|B_n f - f\|_\infty \leq \epsilon \tag{3.25}$$

3.14 More on interpolation

- We can build a piecewise linear interpolant of f to avoid Burge effect when the number of nodes increases. f is a piecewise line or continuous function also called **finite element interpolant**.
- We can perform interpolation bu cubic splines, which are piecewise cubic function $f \in C^2$
- While the Minmax approximation we used so far is based on $\|\cdot\|_\infty$, the least squares approximation uses the Euclidean norm $\|\cdot\|_2$ to minimize $MSE = \sum_{i=0}^{n}(y_i - \tilde{f}(x_i))^2$
- Piecewise linear and splines are well suited to approximate data and functions in several dimensions.
- Trigonometric interpolation is well suited to approximate periodic functions. $\tilde{f}$ is a linear combination of sin and cos functions. FFT and IFFT allow for efficient computation of Fourier coefficients for a trigonometric interpolant from node values.

Chapter 4

Best Approximation in Hilbert spaces

$\mathcal{L}^2$ is an Hilbert space where the norm induced by the scalar product between vectors is $\|x\|_{\mathcal{L}^2} = (x_1^2 + x_2^2 + ... + x_n^2)^{\frac{1}{2}} = \sqrt{(x,x)}$

$$(a,b),\ a,b \in \mathcal{L}^2([0,1]) = \int_0^1 a \cdot b,\ \|a\| = \sqrt{\int_0^1 a^2} \tag{4.1}$$

4.1 Best approximation theorem in $\mathcal{L}^2$

Given a function $f \in \mathcal{L}^2(\mathbb{P}^n)$, p is B.A. of f in $\mathbb{P}^n$ iff

$$(f-p,q) = 0 \quad \forall q \in \mathbb{P}^n,\ \forall f \in \mathcal{L}^2(\mathbb{P}^n) \tag{4.2}$$

(recall: $\|p-f\| \leq \|q-f\|\ \forall q \in \mathbb{P}^n$ if p is B.A. of f w.r.t. chosen norm.)

Proof. Knowing that p is B.A.

$$\|q-f\|^2 = \|q-p+p-f\|^2 = \|q-p\|^2 + \|p-f\|^2 + \underbrace{2(q-p,p-f)}_{0 \text{ since } p-q=q\in\mathbb{P}^k} \text{ and } (0,n) = 0$$

$$\Rightarrow \|p-f\|^2 \leq \|q-f\|^2 \forall q \in \mathbb{P}^n$$

□

Or alternatively, we can

Proof. Knowing that $(f-p,q) = 0 \Rightarrow \|p-f\|^2 \leq \|p-f+tq\|$ with $t \geq 0$ perturbation,

$q \in \mathbb{P}^n$

$$\begin{aligned}
\left\| \underbrace{p - f + \frac{tg}{2}}_{A} \underbrace{- \frac{tg}{2}}_{-B} \right\|^2 \leq & \left\| \underbrace{p - f + \frac{tg}{2}}_{A} + \underbrace{\frac{tg}{2}}_{+B} \right\|^2 \\
0 \leq & 4\Big(p - f + \frac{tg}{2}, \frac{tg}{2}\Big) \\
0 \leq & t^2 \|q\|^2 + 2t(p - f, q) \\
\Rightarrow (p - f, q) \geq & -\frac{t}{2}\|q\|^2
\end{aligned}$$

By choosing $-q$ instead, we get $(p - f, q) \leq \frac{t}{2}\|q\|^2$.
Thus, it is valid $\forall t, \forall q$ that

$$-\frac{t}{2}\|q\|^2 \leq (p - f, q) \leq \frac{t}{2}\|q\|^2 \tag{4.3}$$

which implies that $(p - f, q) = 0$ since a t can be chosen to bound it on both sides.
Since $(p - f, q) = 0 \ \forall q \Leftrightarrow (p - f, v_i) = 0 \ \forall i = 0, 1, ..., n$ with $\mathbb{P} = span\{v_i\}$

$$\Rightarrow (p, v_i) = (f, v_i) \Rightarrow (\sum_{j=0}^{n} p_j v_j, v_i) = (f, v_i) \tag{4.4}$$

□

Computing integrals is easier than performing interpolation, and it yields better results.

4.2 Matrix formulation

We can rewrite $(\sum p_j v_j, v_i) = (f, v_i)$ as a matricial relation

$$Mp = F \text{ where } M_{ij} = (v_j, v_i) = \int_0^1 v_j v_i \text{ and } F_i = (f, v_i) = \int_0^1 f v_i \tag{4.5}$$

If we set $v_i = x^{(i)}$, we obtain the Hilbert matrix

$$M_{ij} = \int_0^1 x^{(j)} x^{(i)} = \frac{1}{i + j + 1} \tag{4.6}$$

The conditional number of the Hilbert matrix is

$$K(M) = O\Big(\frac{(1 + \sqrt{2})}{\sqrt{n}}\Big)^{4n} \tag{4.7}$$

When n increases K explodes, which is very bad. M is difficult to invert and very ill-conditioned because of collinear lines. We would like $M_{ij} = I$, so we use the Legendre basis function to make it orthonormal w.r.t. $\mathcal{L}^2$.

We want $v_i \in \mathcal{P}^n$ s.t. $M_{ij} = (v_i, v_j) = \delta_{ij}$. To build it, we use the Graham-Schmidt method

$$\begin{cases} v_0 = 1, \quad f \ s.t. \ \int_0^1 f = 1 \\ f^{i+1} = x^{i+1} - \sum_{j=0}(x^{(i+1)}, v_j) \\ v_{i+1} = \frac{f^{i+1}}{\|f^{i+1}\|} \end{cases} \tag{4.8}$$

The first line is set of additive basis having unity as first element. This ensures orthogonality between basis function.
As i (the degree) increases, $v_{i+1} = \frac{f^{i+1}}{\|f^{i+1}\|} \to \infty$ since $x^{i+1} \to \infty$
We can avoid instability by using $v_{i+1} = \frac{f_{i+1}}{f_{i+1}(0)}$ instead.
The points created with Graham-Schmidt represent the Legendre Basis. They make p (best approximation) easy to compute, since M becomes easy to invert and we have a diagonal matrix formed by orthogonal basis

$$p = M^{-1}F \tag{4.9}$$

Chapter 5

Integration

Integration is an operation $f[a,b] \to \mathbb{R}$, defined as

$$I(f) = \int_a^b f(x)dx \tag{5.1}$$

Integration is very expensive from a numeric point of view if f is complicated. Our purpose is to make it simpler, given $f \in C^0([a,b])$.
Many possible approaches called quadratures

- Midpoint formula (degree 1)

$$I_{mp}(f) = (b-a)f\Big(\frac{a+b}{2}\Big) \tag{5.2}$$

- Trapezoidal formula (degree 1)

$$I_t(f) = \frac{(b-a)}{2}(f(a)+f(b)) \tag{5.3}$$

- Simpson formula (degree 3), using $\mathcal{L}^2 f$

$$I_s(f) = \frac{(b-a)}{6}\Big(f(a)+4f\Big(\frac{a+b}{2}\Big)+f(b)\Big) \tag{5.4}$$

and their composite variations, using M intervals:

- $I^c_{mp} = H\sum_{k=1}^{M} f(\overline{x}_k)$
- $I^c_t(f) = \frac{H}{2}\sum_{k=1}^{M-1} f(x_k) + \frac{H}{2}(f(a)+f(b))$
- $I^c_s(f) = \frac{H}{6}\sum_{k=1}^{M}(f(x_{k-1})+4f(\overline{x}_k)+f(x_k))$
  with $\overline{x}_k = \frac{(x_{k-1}+x_k}{2}$ and $H = \frac{(b-a)}{M}$

Those are all specific cases of a more general quadrature formula

$$I_n(f) = \sum_{i=0}^{n} \alpha_i f(y_i) \tag{5.5}$$

- $\{y_i\}$ are quadrature nodes.
- α_i are the quadrature weights.

We can use $\mathcal{L}^n f \in \mathbb{P}^n$ at nodes y_i as approximation function, to get the interpolatory quadrature formula

$$f_n(x) = \mathcal{L}^n f(x) : I_n(f) = \int_a^b f_n(x)dx = \int_a^b \sum_{i=0}^n \varphi_i(x) f(y_i)dx$$
$$= \sum_{i=0}^n f(y_i) \int_a^b \varphi_i(x)dx \Rightarrow \sum_{i=0}^n \alpha_i f(y_i)$$

with α_i being $\int_a^b \varphi_i(x)dx$.
The degree of accuracy/exactness of a quadrature is the integer r s.t. quadrature using $\mathbb{P}^n$ doesn't produce errors on $I(f)$

$$\max_{M \in \mathbb{N}} I_n(f) = \int f \ \forall f \in \mathbb{P}^r \tag{5.6}$$

Midpoint rule: for f linear function $\in [a, b]$, we can choose y_i as $\alpha_i = \frac{1}{2}b + \frac{1}{2}a$ to cancel out positive and negative approximation. So we approximate exactly $f \in \mathbb{P}^1$ with a constant function ($\mathbb{P}^0$). We have that

$$\left| \int_a^b f(x)dx - f\Big(\frac{b-a}{2}\Big) \right| \leq \frac{\|f''\|_\infty}{3} \Big(\frac{b-a}{2}\Big)^3 = \frac{\|f''\|_\infty}{24} \quad \text{for } [a, b] = [0, 1] \tag{5.7}$$

Since we can see the error depends on the size of the interval, we usually prefer composite quadrature, pasting together intervals through continuity conditions to keep them small.

5.1 Legendre polynomials and max accuracy

Given $m \in \mathbb{N} > 0$, a quadrature formula $\sum_{i=0}^n \overline{\alpha}_i f(\overline{y}_i)$ has degree of accuracy $n + m$ iff it makes use of interpolation and the nodal polynomial $w_{n+1} = \prod_{i=0}^n (x - \overline{y}_i)$ associated to nodes $\{\overline{y}_i\}$ is s.t.

$$\int_a^b w_{n+1}(x)p(x)dx = 0 \quad \forall p \in \mathbb{P}_{m-1} \tag{5.8}$$

The maximum value for m is $n + 1$, achieved when w_{n+1} is proportional to $L_{n+1}(x)$, the Legendre polynomial of degree $n + 1$. Legendre polynomials can be computed recursively as

$$L_0(x) = 1, \quad L_1(x) = x, \quad L_{k+1}(x) = \frac{2k+1}{k+1} x L_k(x) - \frac{k}{k+1} L_{k-1}(x) \tag{5.9}$$

Since L_{n+1} is orthogonal to $\forall L_{\{0,1,...,n\}}$ ($\int_a^b L_{n+1}(x)L_j(x)dx = 0 \ \forall j < n + 1$), we can see why m is bounded at $n + 1$. Thus, the highest degree of accuracy is $2n + 1$, obtained using the **Gauss-Legendre formula**

$$I_{GL} = \begin{cases} \overline{y}_i = \text{roots of } L_{n+1}(x) \\ \overline{\alpha}_i = \frac{2}{(1-y_i^2)(L'_{n+1}(y_i))^2} \end{cases} \qquad i = 0, ..., n \tag{5.10}$$

The related Gauss-Legendre-Lobatto formula includes interval bounds among quadrature points, and has a D.O.A. of $2n-1$.
The interval used for I_{GL} is $\{-1,1\}$, thus the $\overline{y}_i, \overline{\alpha}_i$ yo reconvert to original values for (a,b), use Chebyshev formula.

$$y_i = \frac{a+b}{2} + \frac{b-a}{2}\overline{y}_i, \quad \alpha_i = \frac{b-a}{2}\overline{\alpha}_i \tag{5.11}$$

Proof. Knowing $f \in \mathbb{P}^{n+m}$, we apply quotient theorem for $\mathbb{P}$

$$f(x) = \underbrace{w_{n+1}(x)}_{\in\mathbb{P}^{n+1}}\underbrace{p(x)}_{\in\mathbb{P}^{m+1}} + \underbrace{q(x)}_{\in\mathbb{P}^{n}}$$
$$\int_a^b f(x) = \underbrace{\int_a^b w_{n+1}(x)p(x)dx}_{(*)} + \int_a^b q(x)dx$$

Assuming that $(*)=0$, we get $\int_a^b f(x) = \int_a^b q(x) = I_n(q)$ (quadrature for $q \in \mathbb{P}^n$ is exact since we took $n+1$ nodes).
Knowing $(*)=0$, we want to prove that if D.O.A. is $n+m$, then $(*)=0$

$$I_n(f) = \int f \ \forall f \in \mathbb{P}^{n+m} \to \int_a^b \underbrace{w_{n+1}(x)p(x)}_{\in\mathbb{P}^{n+m}}dx = I_n(w_{n+1}(x)p(x)) \tag{5.12}$$

Since $I_n(w_{n+1}(x)p(x)) = 0$ because $w_{n+1}(y_i) = 0 \ \forall i$, we proved it.
To prove that m is bound at $n+1$, we could replace $p \in \mathbb{P}^{m-1}$, with $w_{n+1}(x)$, obtaining

$$\int_a^b w_{n+1}(x)w_{n+1}(x)dx = 0 \quad \text{for } m \geq n+2$$
$$\Rightarrow w_{n+1}(x) = 0$$

Which is false, because based on false assumption. □

5.2 Peano integration kernel theorem

The **Peano kernel** represents the error we make when integrating a function $g(x) = (x-\theta)_+^k$ for a given θ.

$$K(\theta) = E_x((x-\theta)_+^k) = \int_a^b (x-\theta)_+^k dx - I_n((x-\theta)_+^k) \tag{5.13}$$

with

$$(x-\theta)_+^k = \begin{cases} (x-\theta)^k & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{5.14}$$

Since

$$\int_a^b (x-\theta)_+^k dx = \frac{(x-\theta)^{k+1}}{k+1}\Big|_{x=b} - \underbrace{\frac{(x-\theta)^{k+1}}{k+1}\Big|_{x=a}}_{0 \text{ since } a \leq \theta} \tag{5.15}$$

we have that it doesn't depend on a.
The Peano kernel theorem says that given a quadrature formula of degree α and $f \in C^{k+1}([a,b])$, with $0 \le k \le \alpha$ then

$$|E(f)| \le \frac{1}{k!}\|k\|_2 \left\| f^{(k+1)} \right\|_2 \tag{5.16}$$

(where other norms combination can be $1-\infty$ and $\infty - 1$)

Proof.

$$f(x) = \underbrace{\sum_{i=0}^{k} \frac{f^i(a)}{i!}(x-a)^i}_{\substack{p(x) \text{ Taylor exp. of } f \\ \text{of order } k \text{ around } a}} + \underbrace{\frac{1}{k!}\int_a^b f^{(k+1)(\theta} K(\theta) d\theta}_{r(x) \text{ from P.K.T.}} = p(x) + r(x)$$

$$E(f) = \int f - I_n(f) = \underbrace{\int p - I_n(p)}_{\substack{\text{cancel out because} \\ p \in \mathbb{P}^d, d<k}} + \int r - I_n(r) = \int r - I_n(r)$$

$$\int_a^b r = \int_a^b \frac{1}{k!}\Big(\int_a^b f^{(k+1)}(\theta)(x-\theta)_+^k d\theta\Big)dx = \int_a^b f^{(k+1)}(\theta)\Big(\int_a^b \frac{(x-\theta)_+^k}{k!}dx\Big)d\theta$$

$$I_n(r) = \int_a^b I(f^{(k+1)}(\theta)\frac{(x-\theta)_+^k}{k!}d\theta = \int_a^b f^{(k+1)}(\theta) I\Big(\frac{(x-\theta)_+^k}{k!}\Big)d\theta$$

$$\Rightarrow E(f) = \int_a^b f^{(k+1)}(\theta) E_x((x-\theta)_+^k)\cdot\frac{1}{k!} = \frac{1}{k!}\int_a^b f^{(k+1)}(\theta)K(\theta)d\theta$$

□

5.3 More on numerical integration

- Simpson adaptive formula uses different steplenghts to compute the composite interpolant on the integral reducing the nodes needed.
- Monte Carlo methods approximate the integral of f as a function statistical mean. They usually lead to poor results.

Chapter 6

Linear Systems

A linear system of order n, $n > 0$, is constituted by a given matrix $A_{n\times n} = (a_{ij})$, a given vector $b = (b_j)$ and an unknown vector $x = (x_j)$ that should be found by solving the system.

$$Ax = b \quad \Rightarrow \sum_{j=1}^{n} a_{ij}x_j = b_i, \quad i = 0, ..., n \tag{6.1}$$

The solution exists and is unique iff A is non-singular ($\det(A) \neq 0$) for any vector b.
In principle, we can compute the solution using the Cramer rule, where A_i is the matrix obtained by replacing the $i-th$ column of A by b, by applying **Laplace extension**

$$x_i = \frac{\det(A_i)}{\det(A)}, \quad i = 1, ..., n \tag{6.2}$$

However, this is computationally infeasible since it requires $\approx 3(n+1)!$ operations. We can reduce the computational cost by applying a method from one of the approaches:

- Direct methods: yield system solution in finite steps.
- Iterative methods: require a (theoretically) infinity of steps.

A full matrix linear system cannot be solved in principle under n^2 operations, one for each element of the matrix.

6.1 Direct methods

Let's define

$$U = (u_{ij}) \Rightarrow u_{ij} = 0 \ \forall i, j \ s.t. \ 1 \leq j < i \leq n, \ U \text{ is upper triangular}$$
$$L = (l_{ij}) \Rightarrow l_{ij} = 0 \ \forall i, j \ s.t. \ 1 \leq i < j \leq n, \ L \text{ is lower triangular}$$

If A is non-singular and triangular, we have that

$$\det(A) = \prod_{i=1}^{n} \lambda_i(A) = \prod_{i=1}^{n} a_{ii} \quad \Rightarrow a_{ii} \neq 0 \ \forall i \tag{6.3}$$

6.1.1 LU factorisation

Let $A \in \mathbb{R}^{n \times n}$, and L, U respectively lower and upper triangular s.t.

$$A = LU \quad \text{LU decomposition/factorisation of } A \tag{6.4}$$

Instead of solving a full linear system, e can solve two triangular systems

$$Ax = b \;\rightarrow\; \begin{cases} Ly = b \\ Ux = y \end{cases} \tag{6.5}$$

Since the two systems are triangular, they can be solved applying respectively a forward substitutions algorithm to get x from U.
Both require n^2 operations to complete.

FORWARD	BACKWARD
$y_1 = \frac{1}{l11} b_1$	$x_1 = \frac{1}{u_{nn}} y_n$
$y_i = \frac{1}{l_{ii}} (b_i - \sum_{j=1}^{i-1} l_{ij} y_j), \ \forall i = 2, ..., n$	$x_i = \frac{1}{u_{ii}} (y_i - \sum_{j=i+1}^{n} u_{ij} x_j), \ \forall i = n-1, ..., 1$

6.1.2 Gauss elimination method (GEM)

6.1.3 Memory-space limitations

6.1.4 Pivoting

6.1.5 Precision of direct methods

6.1.6 Other direct methods

6.2 Iterative methods

6.2.1 Constructing an iterative method

6.2.2 Jacobi method

6.2.3 Gauss-Seidel method

6.2.4 Richardson method

6.2.5 Conjugate gradient method

6.2.6 Convergence criteria

6.2.7 Stopping conditions

6.2.8 Choosing the method

Chapter 7

Eigenvalues and eigenvectors

Chapter 8

Ordinary differential equations

Chapter 9

Finite elements and boundary-value problems