MATH 578 Numerical Analysis, Fall 2020

Student Notes

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Abstract

This is just my re-organized notes going through the highlights from the course material for MATH 578 Numerical Analysis, Fall 2020 [1] and the course textbooks. As a computational statistician muggle taking this course for optimization, this notes *might* not suit your needs. As an overview, the first chapter covers up some basics of analytic functions – specifically, Lagrange interpolation (Taylor series expansion is a special case) and minimax polynomials; the second chapter focuses on solving linear systems, which includes Gaussian elimination, LU factorization, QR factorization, with some content on error analysis; the third and fourth chapters are on eigenvalue problems and iterative methods (all eigenvalue problems must be iterative!), they mostly follow from *Numerical linear algebra*, and consisting of QR algorithms, Arnoldi iteration, GMRES and CG. The last section is on quadrature and ODE solvers, where I gave a very brief summery on Chapter 11 of the book *Numerical Mathematics*.

1 Function Evaluation

Basic Computer Arithmetic $\forall a \in \mathbb{Z}$, a *base–β representation* exists for some $\beta \in \mathbb{N} \setminus \{1\}$:

$$a = \pm \sum_{k=0}^{\infty} a_k \beta^k$$

where $0 \le a_k \le \beta - 1$ is defined as the k–th digit of a in base β. And grade-school column sum/difference first carries out *Cauchy sum* or *difference*, which takes sum/difference for each digits; then it recursively perform carrying for addition for borrowing for subtraction. Let

$$n := \max\{k|a_k \neq 0\},\ m := \max\{k|b_k \neq 0\}$$

So a, b will be $n+1$ and $m+1$ digit number. The bit complexity for addition/subtraction will then be $O(n+m+1)$. Column multiplication carries out similarly. However, multiplication can also be done row-wisely: the *Cauchy product*

$$ab = \left(\sum_{i=0}^{\infty} a_i \beta^i\right) \cdot b = \sum_{i=0}^{n} a_i \cdot \beta^i b$$

where $\beta^j b$ is simply shifting digits, and multiplication by a_i can be carried out as column addition. The bit complexity for column multiplication would then be $O(nm+1)$.

As for division algorithm, assume that the quotient is expressed as:

$$q = q_0 + q_{-1}\beta^{-1} + q_{-2}\beta^{-2} + \cdots$$

And let a, b here be positive and normalized. The *partial reminder* refers to the *normalized* reminder obtained in the division process. Two division algorithms for a/b were introduced here: i). *restoring division*: keeping performing subtraction see if the partial reminder goes below 0, and if it goes below 0, "restore" by adding the divisor back to it to prevent negative digits; ii). *non-restoring division*: the idea of non-restoring division is to use generalized digit, e.g. $\{-1, 1\}$ for binary computing, to allow negative sign in a digit, and a conversion back to standard digit will be indeed required *in the end*. To generalize non-restoring division to any radix β, note that the partial reminders are given by:

$$r_{j+1} = \beta r_j - q_{-j} b$$

the above two division processes determine q_{-j} both by subtracting b from βr_j, the difference is for restoring division, $0 \leq q_{-j} < \beta$ gives partial reminder $0 \leq r_{j+1} < b$; for non-restoring division, $-\beta < q_j < \beta$ gives partial reminder $-b \leq r_{j+1} < b$.

However, both of above division algorithms are not efficient – especially not for bignums. WLOG, let a, b be integers here, the idea of *long division* is to determine the quotient by observing the first digit of the divisor and perform restoring division. In comparison, *SRT division* is non-restoring division with normalized divisor and reminder. *Error propagation* describes the idea of computation will alternate (mostly increase) the error of approximation numbers, such as floating point numbers. Usually error propagation is captured upper-boundedly by *conditional number*, e.g. conditional number of summation is

$$\kappa_+(x) = \frac{|x_1| + |x_2| + \cdots + |x_n|}{|x_1 + x_2 + \cdots + x_n|}$$

Furthermore, the following axiom is used for a wide-range of numerical error analysis for floating point numbers: For each $\star \in \{+, -, \times, /\}$, there exists a binary operation $\circledast$: $\tilde{\mathbb{R}} \times \tilde{\mathbb{R}} \mapsto \tilde{\mathbb{R}}$ s.t.

$$\left| x \star y - x \circledast y \right| \leq \varepsilon \left| x \star y \right|,\ x, y \in \tilde{\mathbb{R}}$$

dividing by zero is excluded. Normally, ε is referred as “machine precision.”

Evaluation of Power Series A function $f : (a,b) \mapsto \mathbb{R}$ is called *analytic* at $c \in (a,b)$ if it can be developed into a power series around c; and called analytic at (a,b) if analytic at c, $\forall c \in (a,b)$. For such class of analytic functions, a way to evaluate them is through Taylor series, backed by a generalized version of mean value theorem proposed by Lagrange: Let f be a $n+1$ times differentiable function in (c,x), with $f^{(n)}$ continuous in $[c,x)$. Then $\exists \xi \in (c,x)$ s.t.

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}$$

See Lagrange interpolation section coming later for proof. This theorem gives an expression of the error as a result of approximating using n–th order Taylor series. Moreover, recall that the *relative condition number* is defined by:

$$\kappa := \lim_{\varepsilon \downarrow 0} \sup_{\|\delta x\| \leq \varepsilon} \frac{\|\delta f\| / \|f(x)\|}{\|\delta x\| / \|x\|}$$

then the following power series are listed with their relative condition numbers:

$$\begin{aligned}
\frac{1}{1-x} =& \sum_{k=0}^{\infty} x^k, \ \forall |x| < 1 \\
\kappa(x) =& \left| \frac{(1-x)^{-2}}{(1-x)^{-1}/x} \right| = \left| \frac{x}{1-x} \right| \\
e^x =& 1 + x + \frac{x^2}{2} + \cdots + \frac{x^n}{n!} + \cdots, \ \forall x \in \mathbb{R} \\
\kappa(x) =& \left| \frac{(e^x)'}{e^x/x} \right| = |x| \\
\log(1+x) =& \sum_{k=1}^{\infty} \frac{(-1)^{n-1} x^n}{k}, \ -1 < x \leq 1 \\
\kappa(x) =& \left| \frac{(1+x)^{-1}}{\log(1+x)/x} \right| = \frac{x}{(1+x)} \cdot \left| \frac{1}{\log(1+x)} \right| \\
\sin x =& \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!}, \ \forall x \in \mathbb{R} \\
\kappa(x) =& \left| \frac{\cos x}{\sin x / x} \right| = |x \cot x| \\
\cos x =& \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!}, \ \forall x \in \mathbb{R} \\
\kappa(x) =& \left| \frac{-\sin x}{\cos x / x} \right| = |x \tan x| \\
\arctan x =& \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{2n+1}, \ |x| \leq 1 \\
\arcsin x =& x + \frac{1}{2} \cdot \frac{x^3}{3} + \frac{1 \cdot 3}{2 \cdot 4} \cdot \frac{x^5}{5} + \frac{1 \cdot 3 \cdot 5}{2 \cdot 4 \cdot 6} \cdot \frac{x^7}{7} + \cdots, \ -1 \leq x < 1
\end{aligned}$$

Acceleration of Convergence Two methods of acceleration of convergence are discussed here:

i). *Euler transform*: *Hausdorff moment characterization theorem* says that (margin here too narrow to contain a good proof)

$$m_k := \int_0^1 x^k d\mu \text{ for some } \sigma\text{-additive Borel probability measure } \mu$$
$$\Leftrightarrow m_0 = 1, \text{ and } m \text{ is completely monotone; i.e., } \forall n,k \geq 0,\ (-1)^n \Delta^n m_k \geq 0$$

Note the recursive definition $\Delta^n m_k := \Delta^{n-1} m_{k+1} - \Delta^{n-1} m_k$ in above formula. Meanwhile, the formula to numerically evaluate π given as

$$\frac{\pi}{4} = \sum_{k=0}^{n} (-1)^k \frac{1}{2k+1}$$

can be accelerated by repeatedly taking average of two consecutive terms, called *Euler transform*. Applying Hausdorff moment characterization, error analysis for this can be done by noticing that

$$a_k = \frac{1}{k} = \int_0^1 t^k d\mu$$

and the rest follows from power series.

ii). *Aitken's Δ^2–process*: used to evaluate a noisy geometric series. For a series defined by

$$a_k = Cq^k + O\left(\delta^k\right), \text{ for some } 0 < \delta < q < 1$$
$$S_n = \sum_{k=1}^{n} a_k$$

Observe that

$$\begin{aligned} S =& S_n + \sum_{k=n+1}^{\infty} a_k \\ =& S_n + \sum_{k=n+1}^{\infty} Cq^k + O(\delta^n) \\ =& S_n + \frac{Cq^{n+1}}{1-q} + O(\delta^n) \end{aligned}$$

$$=S_n + \frac{a_n^2}{a_{n-1} - a_n} + O(\delta^n)$$

The last equality above used the fact that

$$\begin{aligned}
q =& \frac{a_n}{a_{n-1}} + O\left(\left(\frac{\delta}{q}\right)^n\right)\\
a_n =& Cq^n + O(\delta^n)\\
\Rightarrow& Cq^{n+1} = \left(\frac{a_n}{a_{n-1}} + O\left(\left(\frac{\delta}{q}\right)^n\right)\right)(a_n - O(\delta^n)) = \frac{a_n^2}{a_{n-1}} + O(\delta^n), \text{ and}\\
&\frac{1}{1-q} = \frac{a_{n-1}}{a_{n-1} - a_n} + O\left(\left(\frac{\delta}{q}\right)^n\right)
\end{aligned}$$

Let

$$\begin{aligned}
\Delta S_{n-1} :=& S_n - S_{n-1} = a_n\\
\Delta^2 S_{n-2} :=& a_n - a_{n-1} = \Delta a_{n-1}
\end{aligned}$$

We then have the easy-to-compute form for S:

$$S_n + \frac{a_n^2}{a_{n-1} - a_n} = S_n - \frac{(\Delta S_{n-1})^2}{\Delta^2 S_{n-2}}$$

which gives the name "Δ^2"

Root Finding Fixed point iterations are based on a theorem: Let $\phi : (a,b) \mapsto (a,b)$ be continuous. Further, let $x_{k+1} = \phi(x_k)$, $x_0 \in (a,b)$, and

$$\forall x, y \in (a,b),\ \exists \rho < 1 \text{ s.t. } \left|\phi(x) - \phi(y)\right| \leq \rho \left|x - y\right|$$

Moreover, assume that $\exists \alpha \in (a,b)$ s.t. $\phi(\alpha) = \alpha$. Then $\forall x_0 \in (a,b)$, $x_n \to \alpha$ as $n \to \infty$ (linear convergence). Note that possible underlying connection to Lipschitz continuity here. And recall that much of optimization can be more or less considered as a root finding procedure of the first-order optimality condition. The examples given in class are chord method (corresponding to gradient descent), and Newton-Raphson method (local quadratic convergence).

Lagrange Interpolation The problem *Lagrange Interpolation* aims to solve is, given $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$, find coefficients $a_0, \ldots, a_n$ for $p \in \mathbb{P}_n$ s.t.

$$p(x) := \begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & & & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}$$

One way to get the coefficients for the polynomial is to use *Lagrange coefficients*:

$$\phi_k(x) := \prod_{i=0,\ i \neq k}^{n} \frac{x - x_i}{x_k - x_i}$$

and we can construct $p(x)$ this way:

$$p(x) = \sum_{k=0}^{n} y_k \phi_k(x)$$

as it can be observed that

$$\phi_j(x_i) = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Now define *Lagrange interpolation* as a map $\mathcal{L}_n : \mathcal{C}(a, b) \mapsto \mathbb{P}_n$, where $\{x_0, \ldots, x_n\} \subset (a, b)$ are distinct and fixed; i.e., to take $n + 1$ points on f and construct the Lagrange polynomial passing through these $n + 1$ points. Note that $\mathcal{L}_n$ is a *projection*, i.e. $\mathcal{L}_n \mathcal{L}_n = \mathcal{L}_n$. Recall we have mentioned Lagrange's generalization of mean value theorem to higher-orders for Taylor series in evaluation of power series section, and here is its origin – *Lagrange Theorem*:

Let f be $n + 1$th order differentiable in (a, b), and $x \in (a, b)$. Then $\exists \xi := \xi(x)$ s.t.

$$\min\{x_0, \ldots, x_n, x\} < \xi < \max\{x_0, \ldots, x_n, x\}, \text{ and} \tag{1}$$

$$f(x) - (\mathcal{L}_n f)(x) = \frac{(x - x_0) \cdots (x - x_n)}{(n + 1)!} f^{(n+1)}(\xi)$$

i.e., the idea is, existence of a point ξ on $\operatorname{int}(\operatorname{conv}\{x_0,\dots,x_n,x\})$ s.t. the Lagrange interpolation can have an error of power $n+1$. The idea of proof is to construct the *Lagrange reminder*:

$$R(x) := f(x) - (\mathcal{L}_n f)(x);\ A := \frac{R(x)}{\prod_{i=0}^n (x-x_i)}$$

then the function

$$F(z) := f(z) - (\mathcal{L}_n f)(x) - A\prod_{i=0}^{n}(z-x_i)$$

has $n+2$ distinct zeros at $\{x_0,\dots,x_n,x\}$; $F'(z)$ has $n+1$ distinct zeros; ...; $F^{(n+1)}(\xi) = f^{(n+1)}(\xi) - A(n+1)! = 0$ for some ξ in the convex hull as described in (1). This then implies that

$$f(x) - (\mathcal{L}_n f)(x) = R(x) = A\prod_{i=0}^{n}(x-x_i) = \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi)$$

Note here how Rolle's theorem is used to bridge the gap between higher-order in the last of the proof. Another noteworthy thing is that, Taylor's series expansion can be considered as Lagrange interpolation with repeated x_j.

Runge's Phenomenon *Runge's phenomenon* refers to the phenomenon that for a typical analytic function, *equispaced* Lagrange interpolation tends to oscillate more towards the boundary – that is, it tends to interpolate better in the middle. A typical analytic function will have $f^{(n)}(x) \sim \frac{n!}{\delta^n}$, and will have error$\sim \frac{\pi(x)}{\delta^n}$ for $\pi(x) = (x-x_0)\cdots(x-x_n)$. This suggests that *high-order polynomials on equispaced grid is not a good idea*, rather, it's a better idea to pick more points around the edge. Alternatively, it might be a better idea to approximate a function not by interpolating at certain points, but rather to minimize the upper bound of the approximation error norm – which leads to the discussion of the following three sections.

Weierstrass Approximation Theorem The *Weierstrass Approximation Theorem* states that a polynomial is dense in the space of continuous function in uniform norm: Let

$f \in \mathcal{C}[a,b]$ and $\varepsilon > 0$; then $\exists n \in \mathbb{N}$, $\exists q \in \mathbb{P}_n(x)$ s.t.

$$\max_{x\in[a,b]} |f(x) - q(x)| \le \varepsilon$$

Bernstein proposed a constructive proof back in 1904. WLOG, $[a,b] = [0,1]$. Define *Bernstein polynomials* to have coefficients

$$\beta_{n,j}(x) := \binom{n}{j} x^j (1-x)^{n-j},\ j = 0,\dots,n$$

i.e., binomial polynomial if you study stats... It has a few simple but useful properties:

1. $\beta_{n,j}(x) > 0,\ \forall x \in (0,1)$
2. $\sum_{j=0}^{n} \beta_{n,j}(x) = 1$
3. $\sum_{j=0}^{n} \frac{j}{n}\beta_{n,j}(x) = x$
4. $\sum_{j=0}^{n} \frac{j^2}{n^2}\beta_{n,j}(x) = \left(1 - \frac{1}{n}\right)x^2 + \frac{1}{n}x$

And the interpolation proceeds as: let $x_j := \frac{j}{n}$, $j = 0,1,\dots,n$, and let $B_n f(x) := \sum_{j=0}^{n} f\left(x_j\right)\beta_{n,j}(x)$. Then observe that

$$\begin{aligned} f(x) - B_n f(x) &= f(x)\sum_{j=0}^{n}\beta_{n,j}(x) - \sum_{j=0}^{n} f\left(x_j\right)\beta_{n,j}(x) \\ &= \sum_{j=0}^{n}\left[f(x) - f\left(x_j\right)\right]\beta_{n,j}(x) \end{aligned}$$

Now split the function into two components:

$$\begin{aligned} R_\delta(x) &:= \left|\sum_{\left|x-x_j\right|\le\delta}\left[f(x) - f\left(x_j\right)\right]\beta_{n,j}(x)\right| \\ &\le \underbrace{\left|\sum_{j=0}^{n}\beta_{n,j}(x)\right|}_{=1} \cdot \underbrace{\max_{y\in[0,1],\ \left|x-y\right|\le\delta}\left|f(x) - f(y)\right|}_{=:\omega(\delta)} \end{aligned}$$

$$S_\delta(x) := \left| \sum_{|x-x_j|>\delta} \left[f(x) - f\left(x_j\right) \right] \beta_{n,j}(x) \right|$$

and construct interpolation sequence of $\xi_1, \xi_2, \ldots, \xi_p$ between x and x_j s.t. the distance (in Euclidean norm) between two neighbor points $\leq \delta$, then

$$\begin{aligned}
\left| f(x) - f\left(x_j\right) \right| &\leq |f(x) - f(\xi_1)| + |f(\xi_1) - f(\xi_2)| + \cdots + \left| f\left(\xi_p\right) - f\left(x_j\right) \right| \\
&\leq (p+1)\,\omega(\delta) \\
&\leq \left(1 + \frac{\left|x - x_j\right|}{\delta} \right) \omega(\delta)
\end{aligned}$$

This further implies that

$$|S_\delta(x)| \leq \underbrace{\sum_{|x-x_j|>\delta} \omega(\delta)\,\beta_{n,j}(x)}_{\leq \omega(\delta)} + \frac{\omega(\delta)}{\delta} \underbrace{\sum_{|x-x_j|>\delta} \left|x - x_j\right| \beta_{n,j}(x)}_{=:A} \leq \left(1 + \frac{1}{4\delta^2 n} \right) \omega(\delta)$$

where above inequality uses the fact that

$$\begin{aligned}
\delta A &\leq \sum_{|x-x_j|>\delta} \left(x - x_j\right)^2 \beta_{n,j}(x) \\
&\leq \sum_{j=0}^{n} \left(x - x_j\right)^2 \beta_{n,j}(x) \\
&= x^2 \sum_{j=0}^{n} \beta_{n,j}(x) - 2x \sum_{j=0}^{n} \frac{j}{n} \beta_{n,j}(x) + \sum_{j=0}^{n} \frac{j^2}{n^2} \beta_{n,j}(x) \\
&= x^2 - 2x^2 + \left(1 - \frac{1}{n}\right) x^2 + \frac{1}{n} x \\
&= \frac{x(1-x)}{n} \\
&\leq \frac{1}{4n}
\end{aligned}$$

Hence,

$$|f(x) - B_n f(x)| \leq \left(2 + \frac{1}{4n\delta^2} \right) \omega(\delta), \ \forall \delta > 0 \text{ and } x \in [0,1]$$

Pick $\delta = \frac{1}{\sqrt{n}}$ completes the proof.

Minimax polynomials The *minimax polynomial* refers to the polynomial of a given degree that minimizes the uniform norm of the error for a continuous function on a closed interval, and its existence is ensured by the following theorem: Let $f \in \mathcal{C}[0,1]$ and $n \in \mathbb{N}_0$. Then $\exists p \in \mathbb{P}_n$ s.t.

$$\|f-p\|_\infty = \inf_{q\in\mathbb{P}_n} \|f-q\|_\infty$$

such q is called a *minimax polynomial* of degree n for f (on $[0,1]$).

The proof follows from continuous function attains its minimizer over a compact set (Weierstrass Theorem): For the sake of simplicity, let $a \in \mathbb{R}^{n+1}$ denote the coefficient vector for a nth order polynomial q, and

$$E(a) := \|f-q\|_\infty = \max_{x\in[0,1]} |f(x) - q(x)|$$

First we are to prove the continuity of E:

$$\begin{aligned} |E(a+\delta a)| &\le \Big| \|f-q-\delta q\|_\infty - \|f-q\|_\infty \Big| \\ &\le \|\delta q\|_\infty \\ &\le |\delta a_0| + \cdots + |\delta a_n| \end{aligned}$$

Now let $K := \left\{ a \in \mathbb{R}^{n+1} | E(a) \le \|f\|_\infty + 1 \right\}$. Then:

1. *K is closed*, because $K = E^{-1}\left([0, \|f\|_\infty + 1]\right)$ (pre-image of a closed set under continuous mapping is closed)

2. *K is bounded*, because $\|q\|_\infty \le \underbrace{\|f-q\|_\infty}_{=:E(a)} + \|f\|_\infty$ and

$$\|a\| \le \text{constant} \cdot \|q\|_\infty \Rightarrow E(a) \to \infty \text{ as } \|a\| \to \infty$$

3. *Nonempty*, because $0 \in K$

Thus, by Weierstrass Theorem, $\exists a^* \in K$ s.t. $E(a^*) = \inf_{a\in K} E(a)$ – but we still have to prove that $E(a^*) = \inf_{a\in\mathbb{R}^{n+1}} E(a)$:

$$E(a^*) \le E(0) = \|f\|_\infty \le \|f\|_\infty + 1 < E(a),\ \forall a \in \mathbb{R}^{n+1} \setminus K$$

Equioscillation Theorems Two important theorems are given to characterize minimax polynomials.

The first one is *De la Vallee Poussin Theorem*: $\forall f \in \mathcal{C}[a,b],\ n \in \mathbb{N}_0,\ p \in \mathbb{P}_n$, if

$$f\left(x_j\right) - p\left(x_j\right) = (-1)^j e_j,\ \forall j = 0, 1, \ldots, n+1$$

where $a_0 \le x_0 < x_1 < \cdots < x_{n+1} \le b$, and $\operatorname{sgn} e_j = \text{constant}$ for $j = 0, 1, \ldots n+1$; then[1]

$$E_n(f) := \min_{q \in \mathbb{P}_n} \|f - q\|_\infty \ge \min_j \left|e_j\right|$$

i.e., *for a nth order polynomial p oscillates around f with intersecting f for* $n+1$ *times, the uniform norm of the minimax polynomial q is greater or equal to* $\min_j \left|e_j\right|$. The proof is by contradiction: assume that the conclusion is false, then the difference of two nth order polynomials at $x_0, x_1, \ldots, x_{n+1}$ satisfies

$$p\left(x_j\right) - q\left(x_j\right) = (-1)^j e_j + \underbrace{f\left(x_j\right) - q\left(x_j\right)}_{<\left|e_j\right|}$$

$$\Rightarrow p - q \text{ has } n+1 \text{ (distinct) zeros}$$

$$\Rightarrow p \equiv q$$

but it contradicts our assumption on p and q

The second one is *Chebyshev's Oscillation Theorem*, which characterizes the minimax polynomials: $p \in \mathbb{P}_n$ is a minimax polynomial for $f \in \mathcal{C}[0,1]$ iff $f - p$ takes the value $\pm\|f - p\|_\infty$, with alternating changes of sign, at least $n+2$ times in $[0,1]$. Moreover, this minimax polynomial is unique.

For statement besides uniqueness: Proof for "$\Leftarrow$" is done by DLVP, $\|f - p\|_\infty \le E_n(f) \Rightarrow \|f - p\|_\infty = E_n(f)$ by minimality of $E_n(f)$; proof for "$\Rightarrow$" is done by contradiction: assume the conclusion is false, i.e., $f - p$ takes the value $\pm\|f - p\|_\infty$ of k times for some $2 \le k \le n+1$[2],

[1] existence of minimax polynomial was proved in Section 1

[2] $k \ge 2$ because it's a minimax polynomial

and let $\delta := \pm\|f-p\|_\infty$; then $f(x_i)-p(x_i)=(-1)^j\delta$ for $j=1,\ldots,k$. And WLOG this allows us to (quasi-)partition $[0,1]$ into k intervals split by $\xi_1,\xi_2,\ldots,\xi_{k-1}$ s.t. on

$$\begin{aligned}(0,\xi_1),(\xi_2,\xi_3),\cdots &: -\delta \le f-p \le \delta-\varepsilon\\ (\xi_1,\xi_2),(\xi_3,\xi_4),\cdots &: -\delta+\varepsilon \le f-p \le \delta\end{aligned}$$

for some $\varepsilon>0$. Now let $r(x)=\pm(x-\xi_1)\cdots(x-\xi_{k-1})$ – we'll discuss choice of sign shortly after, and let $q(x):=p(x)-\alpha\cdot r(x)$ for some small $\alpha>0$ s.t. $\|\alpha r\|_\infty \le \frac{\varepsilon}{2}$, then $f-q=f-p+\alpha r$. Thus on

$$\begin{aligned}(0,\xi_1),(\xi_2,\xi_3),\cdots &: -\delta < -\delta+\alpha r \le f-q \le \delta-\frac{\varepsilon}{2}\\ (\xi_1,\xi_2),(\xi_3,\xi_4),\cdots &: -\delta+\frac{\varepsilon}{2} \le f-q \le \delta+\alpha r < \delta\end{aligned}$$

and we choose the sign of $r(x)$ s.t. $r>0$ on the first line above and $r<0$ on the second line above. Then q actually takes strictly less error than p, which contradicts that p is the minimax polynomial.

For uniqueness statement: let p,q both be minimax polynomials, and let $r:=\frac{p+q}{2}$. Then

$$\begin{aligned}&|f-r| \le \frac{1}{2}|f-p|+\frac{1}{2}|f-q| \le E_n(f)\\ \Rightarrow&|f-r|=E_n(f) \text{ at } n+2 \text{ distinct points}\\ \Rightarrow&f-p=f-q=\pm E_n(f) \text{ at those points – because } f-p=-(f-q)\Rightarrow f-r=0\\ \Rightarrow&p=q \text{ at } n+2 \text{ distinct points}\\ \Rightarrow&p\equiv q\end{aligned}$$

Chebyshev Polynomials Recall that the Runge's phenomenon suggests that the equispaced interpolation of polynomials does not approximate the function well, then we aim to position the interpolation points over a non-equal grid to approximate the function better. For example, we are to find the minimax polynomial in $\mathbb{P}_n$ for $f(x)=x^{n+1}$. Recall that $\sin,\cos$ usually brings oscillations, but they are not polynomials *per se*, then Chebyshev introduced a polynomial variant from it:

$$t_n(x) := \cos(n\arccos x)$$

which is based on the idea that *the projection of equispaced semi-circle on horizontal axis (see Fig. 1)* – indeed this will put more interpolating points near the boundary. The above polynomial formula gives us $t_n(x) = 1$, $t_1(x) = x$. Recall that

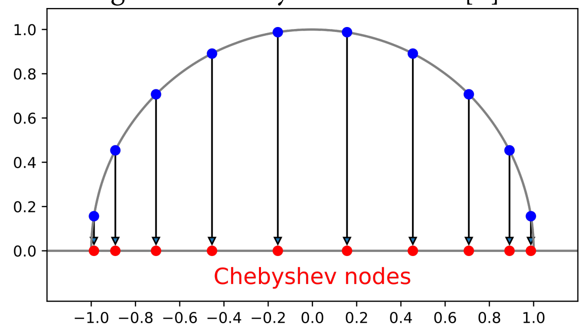
$$\cos((n+1)\theta) + \cos((n-1)\theta) = 2\cos(n\theta)\cos\theta$$

translate this into $t_n(x)$, it is

$$t_{n+1}(x) = 2t_n(x)x - t_{n-1}(x)$$

these are called *Chebyshev polynomials*, the zeros of $t_{n+1}(x)$ satisfy $(n+1)\arccos x = \frac{\pi}{2} + k\pi$ for $k = 0, 1, \dots, n$.

Figure 1: Chebyshev's Nodes [4]



2 Equation Solving

Gaussian Elimination The idea of *Gaussian Elimination* is based on use upper rows to eliminate front-end matrix terms – one term at a time; and the resulting matrix will be an upper-triangular matrix. e.g.:

$$A = \underbrace{\begin{bmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{bmatrix}}_{A_1} \to \underbrace{\begin{bmatrix} 2 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 3 & 5 \end{bmatrix}}_{A_2} \to \underbrace{\begin{bmatrix} 2 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{bmatrix}}_{A_3}$$

written in matrix form of above example, it will be a series of left multiplications:

$$A_2 = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix}}_{\Lambda_1} A_1,\ A_3 = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{bmatrix}}_{\Lambda_2} A_2$$

note that such Λ_k are always lower-triangular – in fact it only has nonzero entries at the kth column and all diagonal entries being 1, as we use upper rows to eliminate elements from lower rows.

LU-decomposition As a summary, for the example in the last section, $A_3 = \underbrace{\Lambda_2\Lambda_1}_{\Lambda} A$; as a product of lower-triangular matrices, Λ is therefore also lower-triangular, hence Λ^{-1} is also lower-triangular. And the decomposition for full rank matrix $A = \Lambda^{-1}A_3$ is called *LU-decomposition*, some useful results in practice:

1. LU-decomposition has arithmetic complexity of roughly $\frac{1}{3}n^3$ multiplications;
2. LU-decomposition breaks down if $(A_k)_{k,k} = 0$ for some k
3. L and U can be stored in a single $n \times n$ array (because Λ^{-1} always has diagonal elements all being 1)

LU decomposition of A exists iff all principal minors of A are nonzero. If exists, LU decomposition is unique. This can be proved by *noticing that Gaussian elimination always preserves principal minors*. For uniqueness, let

$$LU = \hat{L}\hat{U} \Rightarrow \underbrace{\hat{L}^{-1}L}_{\text{lower-trig}} = \underbrace{\hat{U}U^{-1}}_{\text{upper-trig}} = I \Rightarrow \hat{U} = U,\ \hat{L} = L$$

Now the issue still remains if we encounter $(A_k)_{k,k} = 0$ for some k. To solve this issue, and also to make most prominent values (measured by Euclidean norm) up to the top to ensure numerical stability, *pivoting* is introduced. *Partial pivoting* means row interchanges (arithmetic complexity n^2); and *complete pivoting* refers to row and column interchanges (arithmetic complexity $\frac{1}{3}n^3$). An example for partial pivoting row interchange:

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}}_{P} \cdot \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} a_2 \\ a_4 \\ a_1 \\ a_3 \end{bmatrix}$$

and the *permutation matrix* P has properties that $PP^T = P^TP = I$, and the product of permutation matrix is still a permutation matrix (recall it just interchanges rows). Now partial pivoting LU decomposition performs pivoting after each elimination step, specifically,

$$\begin{aligned} U =& \Lambda_n P_n \Lambda_{n-1} P_{n-1} \cdots \Lambda_1 P_1 A \\ =& \Lambda_n \underbrace{\left(P_n \Lambda_{n-1} P_n^{-1}\right)}_{\Lambda'_{n-1}} \underbrace{\left(P_n P_{n-1} \Lambda_{n-2} P_{n-1}^{-1} P_n^{-1}\right)}_{\Lambda'_{n-2}} \cdots \underbrace{\left(P_n \cdots P_2 \Lambda_1 P_2^{-1} \cdots P_n^{-1}\right)}_{\Lambda'_1} P_n \cdots P_2 P_1 A \end{aligned}$$

where $\Lambda'_\cdot$ are *unit lower triangular matrices* – note that they are not lower triangular. And let $\Lambda' = \Lambda_n \Lambda'_{n-1} \Lambda'_{n-2} \cdots \Lambda'_1$, then $U = \Lambda' PA$, this gives

$$PA = LU$$

which is called *PLU-decomposition*. From the above pivoting process, it can be concluded that every square matrix has a PLU-decomposition.

Orthogonalization and QR-decomposition A matrix $Q \in \mathbb{R}^{n\times n}$ is called *orthogonal* if $Q^TQ = I$, i.e., if its column vectors form a orthonormal basis of $\mathbb{R}^n$. The idea of QR-decomposition comes from

$$Ax = QRx = b \Rightarrow QRx = b \Rightarrow Rx = Q^Tb$$

then $Rx = Q^T b$ can be solved by back-substitution. If A, B are orthogonal, then AB and BA are both orthogonal. This allows us to perform QR-decomposition by a series of steps and times an orthogonal matrix at each step.

Recall that the projection of a on b is defined to be

$$\text{proj}_b a := \frac{\langle a, b\rangle}{\|a\| \cdot \|b\|} \cdot \|a\| \cdot \frac{b}{\|b\|} = \frac{\langle a, b\rangle}{\langle b, b\rangle} b$$

First we'll have a look at *Gram-Schmidt method*: let $a_1, a_2, \ldots, a_m \in \mathbb{R}^n$ be column vectors of $A \in \mathbb{R}^{n\times m}$, we can then construct a orthonormal basis for $\text{col}(A)$, denoted by $\{q_1, q_2, \ldots, q_m\}$, by letting

$$\begin{aligned}
&q_1 \leftarrow \frac{a_1}{\|a_1\|};\\
&q_2' \leftarrow a_2 - \langle a_2, q_1\rangle q_1,\ q_2 = \frac{q_2'}{\|q_2'\|};\\
&\vdots\\
&q_m' \leftarrow a_m - \sum_{k=1}^{m-1} \langle a_m, q_k\rangle q_k,\ q_m = \frac{q_m'}{\|q_m'\|}.
\end{aligned}$$

where $\|\cdot\|$ denotes Euclidean norm. i.e., in each Gram-Schmidt step, first take off the projection of a_k onto the existing orthonormal basis we constructed, then the remaining vector will be orthogonal to the existing basis, then normalize a_k. Applying Gram-Schmidt to perform QR-decomposition, each Gram-Schmidt step can be considered as multiplication with a triangular matrix (i.e., step k will normalize $a_k^{(k)}$, and subtract the projections on q_k from $a_{k+1}^{(k)}, a_{k+2}^{(k)}, \ldots, a_m^{(k)}$):

$$\begin{bmatrix} a_1 & a_2 & \ldots & a_m \end{bmatrix}
\begin{bmatrix}
\frac{1}{\langle q_1, a_1\rangle} & -\frac{\langle q_1, a_2\rangle}{\langle q_1, a_1\rangle} & -\frac{\langle q_1, a_3\rangle}{\langle q_1, a_1\rangle} & \cdots & -\frac{\langle q_1, a_m\rangle}{\langle q_1, a_1\rangle}\\
0 & 1 & 0 & & 0\\
0 & 0 & 1 & & 0\\
\vdots & & & \ddots & \vdots\\
0 & 0 & 0 & \cdots & 1
\end{bmatrix}
= \begin{bmatrix} q_1 & a_2^{(2)} & a_3^{(2)} & \ldots & a_m^{(2)} \end{bmatrix}$$

Or view a_k as the sum of its projections on $q_1, q_2, \ldots, q_k$, from which we formulate

$$A = \begin{bmatrix} q_1 & q_2 & \cdots & q_m \end{bmatrix} \begin{bmatrix} \langle q_1, a_1 \rangle & \langle q_1, a_2 \rangle & \cdots & \langle q_1, a_m \rangle \\ 0 & \langle q_2, a_2 \rangle & & \langle q_2, a_m \rangle \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & \langle q_m, a_m \rangle \end{bmatrix} = QR$$

where q_k is obtained using Gram-Schmidt – note that this ensures all the 0s below diagonal.

QR-decomposition by Triangularization *Triangularization* refers to the idea of triangularizing a matrix by zeroing its below-diagonal entries. Here two methods are discussed. The first one is *triangularization by givens rotation*: a *(clockwise) givens rotation matrix*[3] is defined by

$$G = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

And for $a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$, to zero the second entry, i.e., to ensure

$$Ga = \begin{bmatrix} a_1\cos\theta + a_2\sin\theta \\ -a_1\sin\theta + a_2\cos\theta \end{bmatrix} = \begin{bmatrix} \sqrt{a_1^2 + a_2^2} \\ 0 \end{bmatrix}$$

we only need to let

$$\sin\theta = \frac{a_2}{\sqrt{a_1^2 + a_2^2}}$$
$$\cos\theta = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}$$

Note that givens rotation matrix is orthogonal; and generalization to zeroing the $n-$dimensional vector entry a_{k+1} can be simply done by taking an identity matrix and mutate $\begin{bmatrix} I_{kk} & I_{k(k+1)} \\ I_{(k+1)k} & I_{(k+1)(k+1)} \end{bmatrix}$

[3]recall that we have seen them in complex analysis

to be the givens rotation matrix. Then for $A \in \mathbb{R}^{n \times m}$, we can zero the entries of a_i, $\forall i = 1, 2, \ldots, m$ in an order of $n, n-1, \ldots, i+1$ – we have to stop at $i+1$ for a_i as further zeroing will mutate the sparse patterns for zeroed $a_1, a_2, \ldots, a_{i-1}$. This way, we can obtain an upper-triangular matrix.

The second QR-decomposition method is *Householder's reflector*. Different from how givens rotations method *rotates* the vector to zeroing an entry, Householder's method will *reflect* the vector by a hyperplane H s.t. the reflection can point to the desired direction – reflecting one column vector at a time. Specifically, for $a_1 \in \mathbb{R}^n$, we try to reflect a_1 to the direction of e_1 by left-multiplying an orthogonal matrix Q_1 s.t. $Q_1 a_1 = \|a_1\| e_1$, where e_1 denotes the vector with the first entry being 1 and the rest of entries being 0; the hyperplane H is set orthogonal to $v := \|a_1\| e_1 - a_1$, therefore

$$Q_1 = I - 2\frac{vv^T}{v^T v}$$

where Q_1 is orthogonal. In general,

$$Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix}$$

where $I \in \mathbb{R}^{(k-1)\times(k-1)}$, and $F \in \mathbb{R}^{(n-k+1)\times(n-k+1)}$ s.t. $F\tilde{a}_k^{(k)} = \left\|\tilde{a}_k^{(k)}\right\| e_1$, where $\tilde{a}_k^{(k)} \in \mathbb{R}^{n-k+1}$ is $\left(\left(a_k^{(k)}\right)_k, \left(a_k^{(k)}\right)_{k+1}, \ldots, \left(a_k^{(k)}\right)_n\right)$; i.e., the upper-left sub-matrix I together with the two zero sub-matrices are to preserve obtained $a_1^{(k)}, a_2^{(k)}, \ldots, a_{k-1}^{(k)}$ from the first $k-1$ steps, and F is reflecting $\tilde{a}_k^{(k)}$ to obtain $a_k^{(k+1)}$ – which is to be preserved later; i.e., $a_k^{(k+1)} = a_k^{(k+2)} = \cdots = a_k^{(\min(m,n-1))}$.

Singular Value Decomposition (SVD) Click here for the slides I've made for SVD. The most important thing to remember is, *SVD represents a change of basis; i.e., giving adequate basis for domain space and range space, any matrix can be represented as a diagonal matrix.*

Cholesky Decomposition *Hermitian* is an analogue for complex matrices to symmetric for real matrices, defined to be $A = A^*$ if $a_{ij} = \bar{a}_{ji}$. Note that $x^*Ay = \overline{y^*Ax}$ for all $x, y \in \mathbb{C}^m$, this implies $\forall x \in \mathbb{C}^m,\ x^*Ax \in \mathbb{R}$; and it follows that eigenvalues for hermitian matrices are real. If in addition $x^*Ax > 0$ for all $x \neq 0$, then A is called *hermitian positive definite* (note that all positive definite matrices must be hermitian). The eigenvalues for such matrices are all positive – the converse is also true. Eigenvectors corresponding to distinct eigenvalues of a hermitian matrix are orthogonal:

$$\lambda_2 x_1^* x_2 = x_1^* A x_2 = \overline{x_2^* A x_1} = \lambda_1 \overline{x_2^* x_1} = \lambda_1 x_2^* x_2 \Rightarrow x_1^* x_2 = 0$$

Cholesky decomposition on positive definite matrices can be viewed as a *symmetric Gaussian elimination*; i.e., each Gaussian elimination step introduced zeros below the kth entry in column k by left multiplying a matrix, doing this symmetrically on the right will be

$$A = \begin{bmatrix} a_{11} & w^* \\ w & K \end{bmatrix} = \begin{bmatrix} \sqrt{a_{11}} & 0 \\ \frac{w}{\sqrt{a_{11}}} & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & K - \frac{ww^*}{a_{11}} \end{bmatrix} \begin{bmatrix} \sqrt{a_{11}} & \frac{w^*}{\sqrt{a_{11}}} \\ 0 & I \end{bmatrix}$$

and from positive definiteness of A we have $a_{11} > 0$ and $\begin{bmatrix} \sqrt{a_{11}} & 0 \\ \frac{w}{\sqrt{a_{11}}} & I \end{bmatrix}$ is non-singular, which implies $\begin{bmatrix} 1 & 0 \\ 0 & K - \frac{ww^*}{a_{11}} \end{bmatrix} \succ 0$, hence $K - \frac{ww^*}{a_{11}} \succ 0 \Rightarrow$ the upper left corner entry of $K - \frac{ww^*}{a_{11}}$ must be positive. This construction procedure also gives uniqueness of Cholesky factorization.

Conditioning of $Ax = b$ Consider a linear system with numerical error:

$$\begin{aligned} &(A + \delta A)(x + \delta x) = b + \delta b \\ \Leftrightarrow &(A + \delta A)\,\delta x = \delta b - \delta A x \end{aligned}$$

From where, we would expect for all invertible A, $A + \delta A$ will also be invertible if δA is small. To solve this issue, first we'll look at *induced*[4] *matrix norm*, defined for any $A \in \mathbb{R}^{n\times m}$ by

$$\|A\| := \sup_{x\in\mathbb{R}^m} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|\le 1} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|=1} \|Ax\|$$

[4]*induced* means matrix norm induced by vector norms

Immediately following from the definition, the matrix norm satisfies

- $\|\alpha A\| = |\alpha| \|A\|$ (*absolutely homogeneous*)
- $\|A+B\| \leq \|A\| + \|B\|$ (*triangle inequality*)
- $\|A\| \geq 0$ and $\|A\| = 0 \Leftrightarrow A = 0$ (*positive-definiteness*)

and the well-known *Frobenius norm*:

$$\|A\|_F := \sqrt{\sum_{j=1}^{m} \sum_{i=1}^{n} \left|a_{ij}\right|^2} = \operatorname{tr}\left(A^T A\right) = \operatorname{tr}\left(AA^T\right)$$

And another useful fact – *on a finite-dimensional vector space, all norms are equivalent:* for any two norms $\|\cdot\|_a$ and $\|\cdot\|_b$ on finite diemnsional vector space X, $\exists \beta \geq \alpha > 0$ s.t. $\forall x \in X$, $\alpha \|x\|_b \leq \|x\|_a \leq \beta \|x\|_b$.

And for matrix geometric series, we are thinking of

$$(I-K)^{-1} = I + K + K^2 + \cdots \tag{2}$$

and (2) converges iff the $\ell - 2$ norm of all eigenvalues of A are strictly less than 1 – recall that $I-K$ is invertible iff 1 is not an eigenvalue of K. And specific for convergence proof, let

$$B_l := I + K + \cdots + K^l$$

then we have

$$\begin{aligned}\|B_{l+m} - B_l\| &= \left\|K^{l+1} + \cdots + K^{l+m}\right\| \\ &\leq \|K\|^{l+1} + \cdots + \|K\|^{l+m} \\ &\leq \frac{\|K\|^{l+1}}{1 - \|K\|}\end{aligned}$$

if $\|K\| < 1$. Then $\{B_l\}$ is Cauchy, which implies that $\exists B \in \mathbb{R}^{n \times m}$ s.t. $B_l \to B$ as $l \to \infty$.

Now go back to our problem, we need $A + \delta A = A\left(I + A^{-1}\delta A\right)$ to be invertible, then we'll have $(A+\delta A)^{-1} = \left(I + A^{-1}\delta A\right)^{-1} A^{-1}$; and $\left(I + A^{-1}\delta A\right)^{-1}$ exists if $\left\|A^{-1}\delta A\right\| < 1$, note that

$\left\|A^{-1}\delta A\right\| \le \left\|A^{-1}\right\| \|\delta A\|$, then we only need $\|\delta A\| < \frac{1}{\|A^{-1}\|}$. The rest of error analysis follows from matrix norm properties and matrix geometric series properties[5]. Eventually, it can be derived that

$$\frac{\|\delta x\|}{\|x\|} \le \frac{\|A\| \left\|A^{-1}\right\|}{1 - \left\|A^{-1}\delta A\right\|} \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right)$$

where here the *condition number for matrix A* is

$$\kappa(A) = \|A\| \left\|A^{-1}\right\|$$

Backward Error Analysis For floating point addition, we can treat them *as if* the input were perturbed; e.g.:

$$x_1 \oplus x_2 = (x_1 + x_2)(1+\delta) = (1+\delta)x_1 + (1+\delta)x_2 =: \tilde{x}_1 + \tilde{x}_2$$

Applying this treatment to the entire algorithm, we perform *backward error analysis (BEA)*. Let $\tilde{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$ be some algorithmic realization of $f : \mathbb{R}^n \mapsto \mathbb{R}^m$, then BEA refers to the idea of model the errors committed within $\tilde{f}$ by error in the input data. The algorithm $\tilde{f}$ is called *stable* if *it gives nearly the right answer to nearly the right question*; i.e., $\forall x \in \mathbb{R}^n$, $\frac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(\tilde{x})\|} = O(\varepsilon)$ for some $\tilde{x}$ with $\frac{\|\tilde{x}-x\|}{\|x\|} = O(\varepsilon)$. And a stronger condition defined as *backward stable* is used if *the algorithm gives exactly the right answer to nearly the right question*, i.e., $\forall x \in \mathbb{R}^n$, $\tilde{f}(x) = f(\tilde{x})$ for some $\tilde{x}$ with $\frac{\|\tilde{x}-x\|}{\|x\|} = O(\varepsilon)$. The error analysis for an algorithm can be written as

$$\tilde{f}(x) - f(x) = \tilde{f}(x) - f(\tilde{x}) + f(\tilde{x}) - f(x)$$

from which we can deduce that

$$\frac{\left\|\tilde{f}(x) - f(x)\right\|}{\|f(x)\|} \le \frac{\left\|\tilde{f}(x) - f(\tilde{x})\right\|}{\|f(x)\|} + \underbrace{\frac{\|f(\tilde{x}) - f(x)\|}{\|f(x)\|} \cdot \frac{\|x\|}{\|\tilde{x} - x\|}}_{=:\kappa_f(x,\tilde{x})} \cdot \frac{\|\tilde{x} - x\|}{\|x\|}$$

In case of backward stability, we'll have

$$\frac{\left\|\tilde{f}(x) - f(x)\right\|}{\|f(x)\|} \le \kappa_f(x, \tilde{x}) \cdot \frac{\|\tilde{x} - x\|}{\|x\|}$$

[5]which is frequently used when we deal with matrix inverse

Moreover, let $[x,y] := \frac{\|x-y\|}{\|x\|}$ denote some error measure, and we define *backward stability constant of $\tilde{f}$ at x* to be

$$\beta(x) := \inf_{\tilde{x}\in\mathbb{R}^n} \left\{[x,\tilde{x}] \,|\, \tilde{f}(x) = f(\tilde{x})\right\}$$

and backward stability was defined to be $\beta(x) = O(\varepsilon)$. Backward stability can be characterized by the following fact: if $\tilde{f}$ is backward stable at x, then

$$\begin{aligned}\left[f(x), \tilde{f}(x)\right] =& [f(x), f(\tilde{x})] \\ =& \frac{[f(x), f(\tilde{x})]}{\beta(x)} \cdot \beta(x) \\ \leq& \kappa_f(x) \cdot \beta(x) \\ =& O\left(\kappa_f(x) \cdot \varepsilon\right)\end{aligned}$$

Finally, as an example to describe backward non-stability, consider $f : \mathbb{R} \mapsto \mathbb{R}^2$ defined by $f(x) := \begin{bmatrix} \cos x & \sin x \end{bmatrix}^T$, and let $\tilde{f}$ be an algorithm realization of f; but $\tilde{f}(x) \neq f(\tilde{x})$ because the range of f is the unit circle – so unless $\tilde{f}(x)$ maps to a unit circle $\forall x \in \mathbb{R}$, the algorithm $\tilde{f}$ can never be backward stable. It can be shown that naive outer product is not backward stable, and Householder's QR is backward stable.

3 Eigenvalue Problems

Eigenvalue Problems Eigenvalue problems are mostly encountered in iteratively compound form of a matrix, such as power series A^k or e^{tA}. Let X be a matrix with column vectors being eigenvectors of A, then we have

$$AX = X \underbrace{\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_m \end{bmatrix}}_{=:\Lambda} \Rightarrow AX = X\Lambda \Rightarrow A = X\Lambda X^{-1}$$

called the *eigenvalue decomposition* of $A \in \mathbb{C}^{m\times m}$ – it might well not exist. The eigenvalue decomposition can be expressed as a change of basis:

$$Ax = b \Rightarrow \left(X^{-1}b\right) = \Lambda\left(X^{-1}x\right)$$

The set of eigenvectors corresponding to a single eigenvalue forms a subspace of $\mathbb{C}^m$, known as the *eigenspace*, denoted by E_λ; and we have $AE_\lambda \subseteq E_\lambda$. The dimension of E_λ can be interpreted as the maximum number of linearly independent eigenvectors that can be found, defined as the *geometric multiplicity* of λ; recall $\text{null}(A - \lambda I) = E_\lambda$, the geometric multiplicity is then $\dim E_\lambda = \dim(\text{null}(A - \lambda I))$.

The *characteristic polynomial* of $A \in \mathbb{C}^{m\times m}$ is defined as

$$p_A(z) = \det(zI - A)$$

The main usage reflects in the fact that λ is an eigenvalue of $A \Leftrightarrow p_A(\lambda) = 0$. Recall that fundamental theorem of algebra allows us to write $p_A(z)$ as a product of root, which raises the definition of *algebraic multiplicity* of an eigenvalue λ as its multiplicity as a root of p_A.

If $X \in \mathbb{C}^{m\times m}$ is nonsingular, then the map $A \mapsto X^{-1}AX$ is called a *similarity transformation* of A. To characterize similarity transformation, note that if X is nonsingular, then A and $X^{-1}AX$ have the same characteristic polynomial, eigenvalues, as well as algebraic and geometric multiplicities – the rest all follow from characteristic polynomial proof:

$$p_{X^{-1}AX}(z) = \det\left(zI - X^{-1}AX\right) = \det\left(X^{-1}(zI - A)X\right) = \det\left(X^{-1}\right)\det(zI - A)\det(X) = \det(zI - A)$$

and similarity transformation allows us to prove the following proposition: the algebraic multiplicity of an eigenvalue λ is greater or equal to its geometric multiplicity. To see this, for matrix $A \in \mathbb{C}^{m\times m}$, let n be the geometric multiplicity of λ for A, apparently $n \le m$, now form a matrix $V = \begin{bmatrix} \hat{V} & \tilde{V} \end{bmatrix}$, where the column vectors of $\hat{V}$ form a orthonormal basis for E_λ, and $\tilde{V} \in \mathbb{C}^{m\times(m-n)}$ is chosen s.t. V is unitary; then

$$V^*AV = \begin{bmatrix} \lambda I & C \\ 0 & D \end{bmatrix} \tag{3}$$

will have characteristic polynomial $\det(zI-\lambda I)\det(zI-D) = (z-\lambda)^n \det(zI-D)$, which completes the proof.

Note that the geometric and algebraic multiplicity don't have to be the same: e.g., the matrix $\begin{bmatrix} 2 & & \\ & 2 & \\ & & 2 \end{bmatrix}$ and $\begin{bmatrix} 2 & 1 & \\ & 2 & 1 \\ & & 2 \end{bmatrix}$ both have same algebraic multiplicity 3 for eigenvalue $\lambda = 2$, but the former matrix has $\dim E_\lambda = 3$, spanned by e_1, e_2, e_3; the later one, however, has $\dim E_\lambda = 1$, spanned only by e_1. An eigenvalue whose algebraic multiplicity exceeds geometric multiplicity is called a *defective eigenvalue*; and a matrix that has a defective eigenvalue is called a *defective matrix*. The following diagonalization proposition characterizes non-defectiveness: a matrix A is non-defective if it has an eigenvalue decomposition $A = X\Lambda X^{-1}$; "$\Leftarrow$" can be shown by using the similarity transformation proposition we've shown above, and "$\Rightarrow$" can be shown by constructing X using linearly independency of eigenvectors implied by non-defectiveness. As a side-note, *for both defective and non-defective matrices*, the determinant and trace equal to the product and sum of eigenvalues counted with algebraic multiplicity (proved by using characteristic polynomial).

Note that not all diagonalizable matrices have orthogonal eigenvectors – those who do are called unitarily diagonalizable; i.e., $\exists Q$ unitary s.t. $A = Q\Lambda Q^*$. And matrix A is defined to be *normal* if $A^*A = AA^*$. To characterize normality, A is unitarily diagonalizable $\Leftrightarrow$ A is normal; proof for "$\Rightarrow$" is trivial by substitution, proof for "$\Leftarrow$" can be done by Schur factorization:

A *Schur factorization* of a matrix A is a factorization $A = QTQ^*$ where Q is unitary and T is upper-triangular. Every square matrix A has a Schur factorization; the proof uses induction on the dimension of A: similar to (3), for arbitrary square matrix A, $\exists U$ unitary s.t.

$$U^*AU = \begin{bmatrix} \lambda & B \\ 0 & C \end{bmatrix}$$

assume a Schur factorization VTV^* exist for C, then $Q := U\begin{bmatrix} 1 & 0 \\ 0 & V \end{bmatrix}$ is unitary and $Q^*AQ = \begin{bmatrix} \lambda & BV \\ 0 & T \end{bmatrix}$.

Eigenvalue Algorithms An explicit solving method for eigenvalue problems will be reducing to a root finding problem of its characteristic polynomials – but root finding is in fact an ill-conditioned problem *per se*, so it is not really an ideal approach. Moreover, note that for a monic polynomial

$$p(z) = z^m + a_{m-1}z^{m-1} + \cdots + a_1 z + a_0$$

the roots are in fact the eigenvalues of the matrix

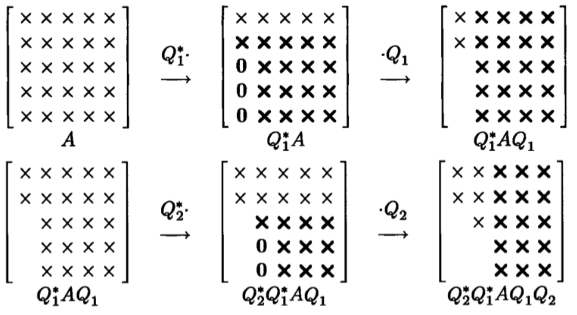
$$A := \begin{bmatrix} 0 & 1 & & & & & \\ & 0 & 1 & & & & \\ & & 0 & 1 & & & \\ & & & \ddots & \ddots & & \\ & & & & 0 & 1 & \\ -a_0 & -a_1 & -a_2 & \cdots & \cdots & -a_{m-2} & -a_{m-1} \end{bmatrix}$$

with corresponding eigenvectors $\left(1, z, z^2, \ldots, z^{m-1}\right)^T$. Therefore, A is called a *companion matrix* corresponding to p. Moreover, Abel proved that no analogue of the quadratic formula can exist for polynomial of degree 5 or more; in view of this, *any eigenvalue solver must be iterative.*

Recall form last section that Schur factorization exists for all matrices, it then follows that most general eigenvalues solver aims to reduce a matrix to by Schur factorization to reveal its eigenvalues. For the sake of computational efficiency, today's algorithms usually splits into two phrases: the first phrase reduce the matrix to a upper–Hessenberg form, and the second phrase upper-triangularizes this upper-Hessenberg matrix.

Now for the first phrase, we apply Householder's reflection to reduce A to a upper-Hessenberg form. At step k, Q_k^* perform Householder's reflection *starting from the second row of the (sub-)matrix* (see the figure), so that right multiplication will not mutate the zeros just created (see Fig. 2).

Figure 2: reduce to upper-Hessenberg form using Householder's reflection [2]



Rayleigh Quotient, Inverse Iteration For this and next section, we consider $A = A^T \in \mathbb{R}^{m \times m}$ and $x \in \mathbb{R}^m$. The *Rayleigh quotient* of a vector $x \in \mathbb{R}^m$ is defined as

$$r(x) := \frac{x^T A x}{x^T x}$$

Apparently, if x is an eigenvector, then $r(x) = \lambda$. The motivation comes from: given x, what scalar α *acts most like an eigenvalue for* x *in the sense of minimizing* $\|Ax - \alpha x\|_2$? Furthermore, we have

$$\nabla r(x) = \frac{2}{x^T x}(Ax - r(x)x)$$

Therefore, at eigenvector x of A, the gradient is a zero vector; moreover, if the gradient is zero at x with $x \neq 0$, then x is an eigenvector and $r(x)$ is the corresponding eigenvalue. Furthermore, note that $\forall \lambda \in \mathbb{R} \setminus \{0\},\ r(\lambda x) = r(x)$; we can then view the Rayleigh quotient as a continuous function on the unit sphere, and its stationary points are normalized eigenvectors of A.

The *power iteration* process can be used to find the eigenvector corresponding to the largest eigenvalue of A: initialized with unit vector $v^{(0)}$, then the update process proceeds as $v^{(k)} \leftarrow$ normalized $Av^{(k-1)}$, and $\lambda^{(k)} \leftarrow \left(v^{(k)}\right)^T Av^{(k)}$.

Recall that the eigenvectors of $(A-\mu I)^{-1}$ are the same as the eigenvectors of A, with corresponding eigenvalues $\left\{\left(\lambda_j-\mu\right)^{-1}\right\}$. Therefore, if choosing μ closer to λ_j than to all other eigenvalues of A, $\left(q_j-\mu\right)^{-1}$ is greater than all other $\left(q_{-j}-\mu\right)^{-1}$; which suggests applying power iteration on $(A-\mu I)^{-1}$ can be used to find eigenvector corresponding to the eigenvalue closest to μ; this process is called *inverse iteration*, which takes updating formula by solving $(A-\mu I)\,w=v^{(k-1)}$ for w and normalize w for $v^{(k)}$.

With a small modification to inverse iteration above: at each step, instead of using μ, we use $r\left(v^{(k-1)}\right)$ – this is called *Rayleigh quotient iteration*.

QR Algorithm The second phrase of eigenvalue problems is based on an algorithm called *QR algorithm* – the idea is based on similarity transformations: initialize $A^{(0)}=A$; for each step, perform QR factorization $Q^{(k)}R^{(k)}=A^{(k-1)}$, then recombine factors $A^{(k)}=R^{(k)}Q^{(k)}$. Under suitable assumptions, it will converge to an upper-triangular form for matrix A – diagonal if A is hermitian. QR algorithm itself is motivated by power iteration; just like inverse iteration can use Rayleigh quotient to for acceleration, same goes for QR algorithm: for step k, we pick a shift $\mu^{(k)}$, then perform QR factorization $Q^{(k)}R^{(k)}=A^{(k-1)}-\mu^{(k)}I$, and recombine factors by $A^{(k)}=R^{(k)}Q^{(k)}+\mu^{(k)}I$. For the choice of shifts, we can choose Rayleigh quotient shift $\mu^{(k)}=R^{(k-1)}_{m,m}$, or Wilkinson's shift, etc.

There are quite a few other algorithms as well; e.g., one might crop the matrix $A^{(k)}$ when $A^{(k)}_{m,m-1}$ becomes close enough to zero, and it turns out to accelerate convergence.

4 Iterative Methods

Iterative Methods Basics Let X be a Banach space and $U\subset X$ be a complete subspace, then $\phi:U\mapsto U$ is called *Lipschitz continuous* if $\exists\rho\geq 0$ s.t. $\left\|\phi(x)-\phi(y)\right\|\leq\rho\left\|x-y\right\|$, $\forall x,y\in U$; furthermore, ϕ is called *non-expansive* if $\rho\leq 1$, and called ρ–contractive if $\rho<1$. As a theorem to characterize ρ–contraction: Let $U\subset X$ be closed, $\phi:U\mapsto U$ be a ρ–contractive mapping, then

- $\exists x \in U$ s.t. $x = \phi(x)$, and x is unique
- $\forall x_0 \in U$, $x_{k+1} = \phi(x_k)$ for $k = 0, 1, \ldots$ converges to x, and

$$\begin{aligned}
\|x_{k+1} - x\| \leq& \rho \|x_k - x\| \\
\|x_k - x\| \leq& \frac{\rho^k}{1-\rho} \|x_0 - x\| \\
\|x_k - x\| \leq& \frac{\rho}{1-\rho} \|x_k - x_{k-1}\|
\end{aligned}$$

we just show the existence and uniqueness of such x in the first point, the rest will be trivial. Note that $\forall n \geq m \geq 1$ and $\forall x_0 \in U$, $\exists \rho < 1$ s.t.

$$\begin{aligned}
\|x_n - x_m\| &= \left\|\phi^n(x_0) - \phi^m(x_0)\right\| \\
&\leq \rho^m \left\|\phi^{n-m}(x_0) - x_0\right\| \\
&\leq \rho^m \left(\left\|\phi^{n-m}(x_0) - \phi^{n-m-1}(x_0)\right\| + \left\|\phi^{n-m-1}(x_0) - \phi^{n-m-2}(x_0)\right\| + \cdots + \left\|\phi(x_0) - x_0\right\|\right) \\
&\leq \rho^m \sum_{i=0}^{n-m-1} \rho^k \left\|\phi(x_0) - x_0\right\| \\
&\leq \rho^m \sum_{i=0}^{\infty} \rho^k \left\|\phi(x_0) - x_0\right\| \\
&= \frac{\rho^m}{1-\rho} \left\|\phi(x_0) - x_0\right\|
\end{aligned}$$

which implies that $\{x_k\}$ is Cauchy. Now let $x \in U$ denote the limit of $\{x_k\}$ as $n \to \infty$, then x is a fixed point because

$$\phi(x) = \phi\left(\lim_{k\to\infty} x_k\right) = \lim_{k\to\infty} \phi(x_k) = \lim_{k\to\infty} x_{k+1} = x$$

and uniqueness of x can be proved by assuming x, y are both fixed points, then

$$0 \leq \left\|x - y\right\| = \left\|\phi(x) - \phi(y)\right\| \leq \rho \left\|x - y\right\| < \left\|x - y\right\|$$

which implies $x = y$.

Here are a few examples of fixed point methods: (i). $\phi(x) = Tx + c$, where T is called *iteration matrix*, contraction of T is equivalent to $\|T\| = \sigma_{\max}(T) \leq 1$. (ii). *Richardson method*:

$\phi(x) = x + \omega(b - Ax)$, where $b - Ax$ is called *residual*. View Richardson's methods in an iteration manner, we have $\phi(x) = (I - \omega A)x + \omega b$; further suppose $A \succ 0$, with eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$, then $I - \omega A$ has eigenvalues $1 - \omega\lambda_1, 1 - \omega\lambda_2, \ldots, 1 - \omega\lambda_n$, then $\|I - \omega A\| = \max_k |1 - \omega\lambda_k| = \max\{|1 - \omega\lambda_1|, |1 - \omega\lambda_n|\}$, which yields the optimal $\omega^* = \frac{2}{\lambda_1 + \lambda_n}$. As a remark to Richardson's method, people usually left-multiply *pre-conditioner* P^{-1} to the linear system, resulting in $P^{-1}Ax = P^{-1}b$ – the purpose here is to make $\operatorname{cond}(A)$ small.

Arnoldi Iteration Most of the iterative methods discussed here will be based on the idea of projecting onto Krylov subspaces. Given matrix $A \in \mathbb{C}^{m\times m}$ and vector b, *Krylov sequence* refers to the set of vectors $b, Ab, A^2b, \ldots$ (they are *not* necessarily linearly independent!), and the corresponding *Krylov subspaces* of order r is then defined as the space spanned by the first r terms of Krylov sequence. *Arnoldi iteration* then can be interpreted as performing (modified) Gram-Schmidt on the Krylov matrix

$$K_n := \begin{bmatrix} b & Ab & A^2b & \cdots & A^{n-1}b \end{bmatrix} \in \mathbb{C}^{m\times n}$$

to construct its orthonormal basis. In view of A itself, Arnoldi iteration can be considered as an Hessenbergized method analogous to Gram-Schmidt, see Table 1 – one similarity is, they both can stop at any iteration with a sequence of triangular/Hessenberg factors and a partial orthogonalized factor $Q^{(k)}$, therefore serves as a better iterative method.

Table 1: Householder's reflection vs Gram-Schmidt/Arnoldi process

	QR factorization $A = QR$	Hessenberg formation $A = QHQ^*$
Householder's reflection	orthogonal triangularization[6]	orthogonal Hessenberg-ition
Gram-Schmidt/Arnoldi process	triangular orthogonalization[7]	Hessenbergized orthogonalization

For iterative methods we consider m to be large or infinite, so we only consider the first n columns of $AQ = QH$. Let $Q_n \in \mathbb{C}^{m\times n}$ denote the first n columns of Q; and let $\tilde{H}_n \in \mathbb{C}^{(n+1)\times n}$ be the submatrix located at the upper-left corner of H, which will also be a Hessenberg matrix itself. Then we'll have $AQ_n = Q_{n+1}\tilde{H}_n$ as the first n columns of $AQ = QH$. *And equating the nth column of both sides gives us* $Aq_n = h_{1n}q_1 + \cdots + h_{nn}q_n + h_{n+1,n}q_{n+1}$, *which is a recurrence relation for* q_{n+1} *– Arnoldi iteration follows directly on this recurrence relation: let* $q_1 = \frac{b}{\|b\|}$ *be the initializer, and choose* h_{kn} *s.t.* $h_{kn}q_k$ *is a projection of* q_k *on* Aq_n *for* $k = 1, 2, \ldots, n$; *as an interpretation, the updating step first subtracts the projections of the built orthogonal bases from* Aq_n, *then normalizing the reminder with* $h_{n+1,n}$ *to ensure* $\|q_{n+1}\| = 1$. Because the recurrence formula states that each q_n is formed by a linear combination of Aq_{n-1} and $q_1, q_2, \ldots, q_{n-2}$, each q_n is therefore a degree-$(n-1)$ polynomial of A times b; hence $q_1, q_2, \ldots, q_n$ form an orthonormal basis for the Krylov subspace

$$\mathcal{K}_n := \left\langle b, Ab, \ldots, A^{n-1}b \right\rangle$$

(i). In this view, Arnoldi process can be considered as systematic construction of orthonormal bases for successive Krylov subspaces $\mathcal{K}_1, \mathcal{K}_2, \mathcal{K}_3, \ldots$. Because Arnoldi iteration constructs orthonormal basis in a Gram-Schmidt manner, the Q_n here will be exactly the same as the Q_n present in the Gram-Schmidt QR factorization of K_n, while here K_n and R *per se* are never explicitly constructed. And it's called *modified* Gram-Schmidt because at iteration k, we subtract projections of constructed bases $q_1, q_2, \ldots, q_k$ from the vector Aq_k instead of the "original" vector $A^k b$.

(ii). Another view of Arnoldi process is a computation of projections onto successive Krylov subspaces. Note that $Q_n^* Q_{n+1}$ is a $n \times (n+1)$ matrix with 1 on the diagonal and 0 elsewhere; then from $AQ_n = Q_{n+1}\tilde{H}_n$ we have

$$\underbrace{Q_n^* Q_{n+1}\tilde{H}_n}_{=:H_n} = Q_n^* A Q_n$$

[6]i.e., (left) multiply an orthogonal matrix in each iteration to triangularize the matrix in the end

[7]i.e.; (right) multiply a triangular matrix in each iteration to orthogonalize the matrix in the end

apparently, H_n here will be the $n \times n$ submatrix located at the upper-left corner of H. This is an analogue to change of basis, with Q_n not orthogonal but of shape $m \times n$ – and the resulting interpretation is: given some $v \in \mathcal{K}_n$, applying A to it, then orthogonally project Av back to $\mathcal{K}_n$.

Note that here H_n and A are *pseudo*-similar. Intuitively, one might then consider the eigenvalues of H_n as estimates for the eigenvalues of A – for this reason, they are called *Arnoldi eigenvalue estimates* (at step n) or *Ritz values* (wrt. $\mathcal{K}_n$).

Consider a vector $x \in \mathcal{K}_n$, such a vector can then be written as a linear combination of Krylov's vectors $b, Ab, \ldots, A^{n-1}b$, put in polynomial form, it will be

$$x = q(A)\,b$$

Now consider $P^n :=$ {monic polynomials of degree n}, the famous *Arnoldi-Lanczos approximation problem* is proposed as

$$\min_{p^n \in P^n} \|p^n(A)\,b\|$$

and the Arnoldi iteration solves this problem exactly (if it doesn't break down ofc...) – *the minimizer $\bar{p}^n$ is uniquely given by the characteristic polynomial of H_n.* As a proof, let $y := A^n b - p^n(A)\,b \in \mathcal{K}_n$, then the problem can be considered as minimizing $\left\|A^n b - y\right\|$ wrt. y; i.e., minimizing the distance from $A^n b$ to $\mathcal{K}_n$ – thus the minimization can be characterized by $p^n(A)\,b \perp \mathcal{K}_n \Leftrightarrow Q_n^* p^n(A)\,b = 0$ as $q_1, q_2, \ldots, q_n$ are a basis of $\mathcal{K}_n$. Now consider $A = QHQ^*$; where $Q := \begin{bmatrix} Q_n & U \end{bmatrix}$ s.t. Q is a orthogonal matrix extended from Q_n, and $H := \begin{bmatrix} H_n & X_2 \\ X_1 & X_3 \end{bmatrix}$, where the entries of X_1 is all 0 besides its upper-right entry and X_3 is Hessenberg – due to the Hessenberg structure of H. Then we have

$$\begin{aligned} & Q_n^* p^n(A)\,b = 0 \\ \Leftrightarrow & Q_n^* Q p^n(H)\,Q^* b = 0 \\ \Leftrightarrow & \begin{bmatrix} I_n & 0 \end{bmatrix} p^n(H)\,e_1 \|b\| = 0 \end{aligned} \tag{4}$$

and (4) follows from $q_1 = \frac{b}{\|b\|}$. The interpretation of last equation is, the minimization characterization now becomes that the first n entries in the first column of $p^n(H)$ are 0. Due to the Hessenberg structure of H, the first n entries in the first column of $p^n(H)$ are exactly the first column of $p^n(H_n)$ – in view of this, it is *sufficient* to make $p^n(H_n) = 0$: by Cayley-Hamilton theorem, if p^n is the characteristic polynomial of H_n, $p^n(H_n) = 0$. Proof of uniqueness uses contradiction: if uniqueness is voided, taking difference of two distinct degree-n monic polynomials that both minimize $\|p^n(A)b\|$ will then result in a non-zero polynomial $q(A)$ of degree $\leq n-1$ s.t. $q(A)b = 0$ – this contradicts the assumption that K_n is of full-rank.

Based on this finding, *(iii). the Ritz values generated by Arnoldi iteration are the roots of the optimal polynomial to the Arnoldi-Lanczos approximation problem.* And this gives the Ritz values some invariant properties:

- *(translation invariance)* If A is changed to $A + \sigma I$ for some $\sigma \in \mathbb{C}$, and b is left unchanged, the Ritz values $\left\{\theta_j\right\}$ at each step will be changed to $\left\{\theta_j + \sigma\right\}$
- *(scale invariance)* If A is changed to σA for some $\sigma \in \mathbb{C}$, and b is left unchanged, the Ritz values $\left\{\theta_j\right\}$ at each step will be changed to $\left\{\sigma\theta_j\right\}$
- *(unitary similarity transformation invariance)* If A is changed to UAU^* for some unitary U, and b is changed to Ub, the Ritz values do not change

GMRES *Generalized minimal residuals (GMRES)* is a method *using Arnoldi iteration to solve a linear system $Ax = b$, the resulting mechanic is to use $x_n \in \mathcal{K}_n$ at step n to approximate the root by formulating the problem:*

$$\begin{aligned}
&\min_{x_n \in \mathcal{K}_n} \|Ax_n - b\| \\
\Leftrightarrow &\min_{c \in \mathbb{C}^n} \|AK_n c - b\| \\
\Leftrightarrow &\min_{y \in \mathbb{C}^n} \left\|AQ_n y - b\right\|
\end{aligned}$$

$$\Leftrightarrow \min_{y\in\mathbb{C}^n} \left\| Q_{n+1}\tilde{H}_n y - b \right\|$$

$$\Leftrightarrow \min_{y\in\mathbb{C}^n} \left\| \tilde{H}_n y - Q_{n+1}^* b \right\| \tag{5}$$

$$\Leftrightarrow \min_{y\in\mathbb{C}^n} \left\| \tilde{H}_n y - \|b\| e_1 \right\| \tag{6}$$

where (5) is because that b is in the column space of Q_{n+1} (because $q_1 := \frac{b}{\|b\|}$), therefore left multiplication of Q_{n+1}^* does not change the norm. Furthermore, note that $Q_{n+1}^* b = \|b\| e_1$, which gives us (6).

On another note, the initial assumption for GMRES of $x_n \in \mathcal{K}_n$ is equivalent to $x_n = q_n(A)\, b$ for some degree-$(n-1)$ polynomial q_n, with coefficients being c mentioned in above equations. Then the residual satisfies $b - Ax_n = (I - Aq_n(A))\, b$; let $p_n(z) := 1 - zq(z)$, then GMRES in fact solves problem $\min_{p_n \in P_n} \|p_n(A)\, b\|$, but with $P_n := \{\text{degree} \le n \text{ polynomials } p \text{ with } p(0) = 1\}$ here.

Lanczos Iteration and CG If A is Hermitian, the Arnoldi iteration will be redundant to find eigenvalues of A – a method called Lanczos iteration was introduced as a simplification of Arnoldi iteration (*mainly simplified by noticing that H_n becomes tri-diagonal now*). With a similar simplification idea, if A is symmetric positive definite, solving $\min_x \|Ax - b\|$ using GMRES will in fact not be efficient – *conjugate gradient (CG)* was then introduced based on *minimizing the A-norm of the error*; where the *A-norm of e_n* $:= x^* - x_n$ is defined as $e_n^T A e_n$. Specifically, the famous CG is proposed as algorithm 1 on the following page.

And induction on n can show that:

1. *(identity of subspaces)*

$$\begin{aligned}\mathcal{K}_n &= \langle x_1, x_2, \ldots, x_n \rangle = \langle p_0, p_1, \ldots, p_{n-1} \rangle \\ &= \langle r_0, r_1, \ldots, r_{n-1} \rangle = \left\langle b, Ab, \ldots, A^{n-1} b \right\rangle\end{aligned}$$

2. *(orthogonal residuals)*

$$r_i^T r_j = 0,\ \forall i \neq j$$

Algorithm 1 Conjugate Gradient (CG)

```
Input: $A \in \mathbb{R}^{m \times m} \succ 0$, $b \in \mathbb{R}^m$
Output: $x_n$ – the solution of linear system $Ax = b$
1: Set $x_0 \leftarrow 0$, $r_0 \leftarrow b$, $p_0 \leftarrow r_0$                ▹ Initialization
2: while not converged do
3:     $\alpha_k \leftarrow \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T A p_{k-1}}$                ▹ calculate step length
4:     $x_k \leftarrow x_{k-1} + \alpha_k p_{k-1}$                ▹ approximate solution
5:     $r_k \leftarrow r_{k-1} - \alpha_k A p_{k-1}$                ▹ calculate residual
6:     $\beta_k \leftarrow \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}$                ▹ calculate improvement from this step
7:     $p_k \leftarrow r_k + \beta_k p_{k-1}$                ▹ calculate next step's search direction
```

3. *(A-conjugate search directions)*

$$p_i^T A p_j = 0,\ \forall i \neq j$$

Following results above, for iteration n, we can show that x_n is the unique point in $\mathcal{K}_n$ that minimizes $\|e_n\|_A$; and the convergence is monotonic (descent property), i.e.,

$$\|e_n\|_A \leq \|e_{n-1}\|_A$$

and $e_n = 0$ is achieved for some $n \leq m$. The first statement follows simple calculation, the monotonicity follows $\mathcal{K}_n \subset \mathcal{K}_{n+1}$.

As CG minimizes A-norm of the error in an iterative manner, this enables us to view CG as an optimization algorithm – simple calculations allow us to formulate the following problem for CG:

$$\min_{x \in \mathbb{R}^m} \frac{1}{2} x^T A x - x^T b$$

Lastly, similar to how we build the connection between Arnoldi iteration and GMRES in a polynomial minimization manner at the end of last section, it's similar for CG: CG approximation problem can be formulated as $\min_{p_n \in P_n} \|p_n(A) e_0\|_A$; where $e_0 := x^* - x_0$ denotes the initial error, and $P_n := \{\text{degree} \leq n \text{ polynomials } p \text{ with } p(0) = 1\}$, same as before.

5 Quadrature and ODE Solvers

Numerical Integration Let $f : \mathbb{R} \mapsto \mathbb{R}$ be a second-order smooth function, i.e., $f \in \mathcal{C}^2$, numerical integration aims to approximate the integral $I(f) := \int_a^b f(x)\,dx$. *Midpoint method* uses the midpoint $c := \frac{a+b}{2}$: based on Taylor theorem $f(x) = f(c) + f'(c)(x-c) + O\left(h^2\right)$, where $h := b-a$; then the midpoint approximation will be $\tilde{I}(f) = (b-a)f\left(\frac{a+b}{2}\right) + O\left(h^3\right)$. *Composite midpoint formula* improved by dividing $[a,b]$ into n intervals, each of length $h := \frac{b-a}{n}$; i.e., consider $n-1$ "midpoint" interpolations $a < x_1 < x_2 < \cdots < x_n < b$; as a result, the error is now $n \cdot O\left(h^3\right) = O\left(n^{-2}\right) = O\left(h^2\right)$.

Now consider when $f \in \mathcal{C}^1$, we are to perform analysis of convergence for the midpoint rule, called *Lebesgue type analysis*. Now consider the integral and approximate-integral operators I and $\tilde{I} : C([a,b]) \mapsto \mathbb{R}$; it's trivial that they are both linear operators. The *degree of exactness* measures to which degree of polynomial p, $\tilde{I}(p)$ approximates $I(p)$ exactly; e.g., for midpoint method, we have $\tilde{I}(p) = I(p)$ for $p \in P_1$, then the degree of exactness is 1. As a normal strategy in numerical analysis, we analyze error by using polynomials:

$$\begin{aligned}\tilde{I}(f) - I(f) &= \tilde{I}(f) - \tilde{I}(p) + I(p) - I(f) \\ &= \tilde{I}(f-p) + I(p-f) \\ &= \left(\tilde{I} - I\right)(f-p)\end{aligned} \tag{7}$$

Now consider the norm of I, defined by $\|I\| = \sup_f \frac{|I(f)|}{\|f\|_\infty}$:

$$\begin{aligned}|I(f)| = \left|\int_a^b f(x)\,dx\right| \le (b-a)\|f\|_\infty \Rightarrow \frac{|I(f)|}{\|f\|_\infty} \le b-a \\ \forall f \text{ constant function, } \left|\int_a^b f(x)\,dx\right| = (b-a)\|f\|_\infty \Rightarrow \sup_f \frac{|I(f)|}{\|f\|_\infty} \ge b-a\end{aligned}$$

therefore, $\|I\| = b-a$; same goes for $\tilde{I}$, we'll have $\left\|\tilde{I}\right\| = b-a$. And from (7),

$$\begin{aligned}&\left|\tilde{I}(f) - I(f)\right| \le \left|\tilde{I}(f-p)\right| + |I(p-f)| \le 2(b-a)\|f-p\|_\infty,\ \forall p \in P_1 \\ \Rightarrow &\left|\tilde{I}(f) - I(f)\right| \le 2(b-a)\inf_{p \in P_1}\|f-p\|_\infty\end{aligned}$$

this analysis essentially says without assumption $f \in \mathcal{C}_2$, the quadrature error can be deduced from p – making p to be the minimax polynomial of f can give most meaningful results (though not always easy). Note that p here is merely a tool introduced to perform error analysis.

In general, quadrature proceeds as

$$\tilde{I}(f) = \sum_{i=0}^{n} w_i f(x_i),\ a \le x_i \le b$$

and the sequence $x_1, x_2, \ldots, x_n$ are called *quadrature nodes*, while $w_1, w_2, \ldots, w_n$ are called *quadrature weights*. An example could be *interpolatory quadrature*, which proceeds by computing the Lagrangian interpolation polynomial first, then taking integral of the polynomial:

$$\begin{aligned}\tilde{I}(f) = I(\mathcal{L}_n f) &= \int_a^b \mathcal{L}_n f(x)\,dx \\ &= \int_a^b \sum_{i=0}^{n} f(x_i)\,\phi_i(x)\,dx \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b \phi_i(x)\,dx\end{aligned}$$

and the degree of exactness here will be at least n – as Lagrangian interpolation can represent a degree-n polynomial exactly. The rest of error analysis will proceed similar as we've seen before for midpoint quadrature.

(first-order[8]) IVP The *initial value problem (IVP)*, otherwisely called the *Cauchy problem*, basically refers to a DE with initial values given; specifically, it is defined as finding a real-valued function $y \in C^1(I)$ s.t.

$$\begin{cases} y'(t) = f(t, y(t)), & t \in I \\ y(t_0) = y_0 \end{cases} \tag{8}$$

[8]Note that in numerical analysis, *first-order IVP* is of special interest because higher-order IVP can always be rewritten as a first-order IVP; e.g. see this example of six-body motion problem (Problem 4) solved by Runge-Kutta.

where $f(t,y)$ is a given real-valued function in the strip $S = I \times \mathbb{R}$. Immediately from this definition, we have the following equivalent of above formula:

$$y(t) - y_0 = \int_{t_0}^{t} f(\tau, y(\tau))\, d\tau$$

And recall from ODE that the existence and uniqueness results are:

1. *Local*: if $f(t,y)$ is locally L–Lipschitz continuous at (t_0, y_0) wrt. y, with the neighborhood J, Σ width to be r_J for t_0 and r_Σ for y_0; then the IVP admits a unique solution in a neighborhood of t_0 with radius $0 < r_0 < \min\left\{r_J, \frac{r_\Sigma}{\max_{t,y\in J\times\Sigma}|f(t,y)|}, \frac{1}{L}\right\}$;
2. *Global*: if f is uniformly Lipschitz continuous wrt. y over the entire domain $I \times \mathbb{R}$.

And in view of stability analysis of IVP, the definition follows from the idea that *small perturbations results in small error to solutions*. Formally, the IVP is *Lyapunov stable on I* if $\forall(\delta_0, \delta(t))$ satisfying

$$|\delta_0| < \varepsilon,\ |\delta(t)| < \varepsilon,\ \forall t \in I,$$

with $\varepsilon > 0$ sufficiently small to ensure existence of solution for the perturbed problem

$$\begin{cases} z'(t) = f(t, z(t)) + \delta(t), & t \in I \\ z(t_0) = y_0 + \delta_0, \end{cases}$$

we have $\exists C > 0$ s.t. $\left|y(t) - z(t)\right| < C\varepsilon,\ \forall t \in I$ – *the constant C here depends on t_0, y_0, f, but not on ε.*

Numerical Methods for ODE The approximation of the problem (8) is called *one-step* method if $\forall n \geq 0$, u_{n+1} depends only on u_n; otherwise, it will be called *multistep* method. Moreover, if u_{n+1} depends only on the past q steps (i.e., $u_n, \ldots, u_{n+2-q}, u_{n+1-q}$). A few one-step methods are:

- forward Euler: $u_{n+1} \leftarrow u_n + hf_n$

- backward Euler: $u_{n+1} \leftarrow u_n + hf_{n+1}$
- Crank-Nicolson method: $u_{n+1} \leftarrow h \cdot \frac{f_n + f_{n+1}}{2}$
- Heun method: $u_{n+1} \leftarrow u_n + h \cdot \frac{f_n + f(t_{n+1}, u_n + hf_n)}{2}$

A method is called *explicit* if u_{n+1} can be computed directly from u_k, for some $k \leq n$ (e.g., forward Euler and Heun); *implicit* if u_{n+1} depends implicitly on itself through f (e.g., backward Euler and Crank-Nicolson).

The *linear multistep method* refers to

$$u_n \leftarrow \sum_{j=1}^{r} a_j u_{n-j} + h\left(\sum_{j=1}^{r} b_j f_{n-j} + b_0 f_n\right), \forall n = r, r+1, \ldots$$

or write in a more interpretable manner: the updating formula above aims to build a connection between numerical values and slopes:

$$u_n - \sum_{j=1}^{r} a_j u_{n-j} = h\left(\sum_{j=1}^{r} b_j f_{n-j} + \underbrace{b_0 f_n}_{\text{implicit term}}\right)$$

Linear multistep method is, of course, linear in both u. and f., and it evaluates f. once per step; its accuracy can be increased by increasing the number of steps r. For the sake of clarity, we shall re-parameterize the equation above, denoted by:

$$\sum_{j=0}^{r} \alpha_j u_{k+j} = h\left(\sum_{j=0}^{r} \beta_j f_{k+j}\right)$$

where now $k := n - r$. Thanks to its simple linear structure, error analysis is feasible for linear multistep method – first let's define the local truncation error for linear multistep method τ_h:

$$h\tau_h := y_{k+r} - u_{k+r}$$

And the error analysis will just assume previous r steps are exact, i.e., $u_{k+j} = y_{k+j}$ for $j = 0, 1, \ldots, r-1$. Under this assumption, the error analysis can be achieved by substitution to the updating formula:

$$\begin{aligned}\alpha_r u_{k+r} + \sum_{j=0}^{r-1} \alpha_j y_{k+j} &= h\left(\beta_r f_{k+r} + \sum_{j=0}^{r-1} \beta_j f\left(t_{k+j}, y_{k+j}\right)\right) \\ &= h\left(\beta_r f_{k+r} + \sum_{j=0}^{r-1} \beta_j y'_{k+j}\right)\end{aligned}$$

and taking difference term-wisely, we have:

$$\begin{aligned}L_h &:= \sum_{j=0}^{r} \left[\alpha_j y_{k+j} - h\beta_j y'_{k+j}\right] \qquad (9) \\ &= \alpha_r \left(y_{k+r} - u_{k+r}\right) - h\beta_r \left(f\left(t_{k+r}, y_{k+r}\right) - f_{k+r}\right) \\ &= \alpha_r \left(y_{k+r} - u_{k+r}\right) - h\beta_r \underbrace{\left[\frac{\partial f}{\partial u}(\xi)\right]}_{=: J \in \mathbb{R}^{m\times m}} \left(y_{k+r} - u_{k+r}\right)\end{aligned}$$

where m is just the dimension of $u_.$ or $y_.$, and the symbol "ξ" comes from mean value theorem. Moreover, by definition, now we have

$$h\tau_n(h) = \left(\alpha_0 I - h\beta_0 J\right)^{-1} L_h$$

The linear multistep method is *of order p* if $\tau_n(h) = O(h^p) \Leftrightarrow L_h = O\left(h^{p+1}\right)$. And from above steps, we are ready to prove that the following statements are equivalent:

1. linear multistep method is of order p
2. $\sum \alpha_j = 0, \sum j\alpha_j = \sum \beta_j, \sum j^2 \alpha_j = 2\sum j\beta_j, \cdots, \sum j^p \alpha_j = p\sum j^{p-1}\beta_j$
3. $\rho\left(e^h\right) - h\cdot\sigma\left(e^h\right) = O\left(h^{p+1}\right)$ as $h \to 0$, where the characteristic and generating polynomials are defined by

$$\begin{aligned}\rho(z) &= \alpha_0 + \alpha_1 z + \cdots + \alpha_r z^r \\ \sigma(z) &= \beta_0 + \beta_1 z + \cdots + \beta_r z^r\end{aligned}$$

4. $\frac{\rho(z)}{\log z} - \sigma(z) = O\left((z-1)^p\right)$ as $z \to 1$

The proof of equivalence between 2 and 3 follows by taking $u(t) = e^t$ we have

$$L_h = \sum_{j=0}^{r} \left[\alpha_j e^{t+jh} - h\beta_j e^{t+jh} \right] = e^t \left[\rho\left(e^h\right) - h \cdot \sigma\left(e^h\right) \right].$$

and other part of proof follows by taking second-order Taylor polynomial expansion on (9).

The *Runge-Kutta method* refers to

$$u_{n+1} \leftarrow u_n + h \cdot F(t_n, u_n, h; f), \ \forall n \geq 0$$

where F is the increment function defined as:

$$\begin{aligned} F(t_n, u_n, h; f) &= b^T K, \\ [K]_i &= f(t_n + [c]_i h, u_n + hA_{i,:}K), \ i = 1, 2, \ldots, s \end{aligned}$$

where $A := \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1s} \\ a_{21} & a_{22} & & a_{2s} \\ \vdots & & \ddots & \vdots \\ a_{s1} & a_{s2} & \cdots & a_{ss} \end{bmatrix} \in \mathbb{R}^{s\times s}$, $b, c \in \mathbb{R}^s$; and we assume $c_i = \sum_{j=1}^{s} a_{ij}$, $\forall i = 1, 2, \ldots, s$.

Obviously Runge-Kutta is explicit iff A is a strictly lower triangular matrix. *Runge-Kutta method is a one-step method, and its accuracy can be increased by increasing number of function evaluations s.* Finally, it's straightforward to verify that both Euler's methods belong to the Runge-Kutta family. From the optimization perspective, forward Euler's method corresponds to gradient descent, while backward Euler's method with Newton-Raphson as the iterative solver and forward Euler as stepwise initial guess behaves like Newton-Raphson – see numerical example here (Problem 2 a.).

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