

# Numerical Analysis Projects : Comprehensive Report

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**Projects done : 3 , 4 , 6 , 7 , 9**

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## Notes :

All the vectors and matrices in the report are denoted by bold letters (e.g.  $\mathbf{A}$ ,  $\mathbf{x}$  etc.). The codes or presentation corresponding to each project is highlighted in green and the file names are mentioned at the end of each project. This document is written using *LaTeX* in Overleaf.

## ✳ Project #3

❖ **Answer :** The maximum likelihood estimator of  $p$  is 0.4795832 .

❖ **Solution :** We need to find a point  $p$  where the function

$$L(p) = p^{46}(q^2 + 2pq)^{77} = p^{46}q^{77}(1 + p)^{77} = p^{46}(1 - p^2)^{77}$$

is maximized, provided that the probability that a parent gives an "a" allele to an offspring is  $p \in [0, 1]$ .

Now,  $L(p)$  is a polynomial in  $p$ , thus continuous and differentiable over  $(0, 1)$ . Also, whenever  $0 < p < 1$ , clearly we have  $0 < L(p) < 1$ .

Now,  $L(0) = L(1) = 0$ , i.e.  $L$  attains its minimum value at both of the endpoints of its domain. So, if any point in  $[0, 1]$ , where  $L$  attains its maximum value, must be strictly inside the open interval  $(0, 1)$ . In fact, we can guarantee the existence of at least one such point because  $L$  is continuous over the closed interval  $[0, 1]$ , henceforth bounded and it must attain its maximum value somewhere in  $(0, 1)$ .

Differentiating  $L$ , we obtain

$$\begin{aligned} L'(p) &= 46p^{45} \cdot (1 - p^2)^{77} - p^{46} \cdot 77(1 - p^2)^{76} \cdot 2p \\ &= p^{45}(1 - p^2)^{76} [46 - 46p^2 - 154p^2] \\ &= 2p^{45}(1 - p^2)^{76} (23 - 100p^2) \end{aligned}$$

In order for  $L(p)$  to maximize, we need  $L'(p) = 0$  at some point. So, we need to solve for  $p$  such that  $f(p) = L'(p) = 0$ . To do this, we employ **Bisection Method**. At first, we find two points  $a_0$  and  $b_0$  such that  $\text{sgn}(f(a_0)) \neq \text{sgn}(f(b_0))$ .


Now, for any  $k = 0, 1, 2, \dots$ , in general, consider  $m_k = \frac{a_k + b_k}{2}$ . If  $f(m_k) = 0$  for some  $k$ , we are done. If not, then we check  $\text{sgn}(f(m_k))$  and find out if it matches with  $\text{sgn}(f(a_k))$  or  $\text{sgn}(f(b_k))$ .

In general, for some  $k \in \mathbb{N}$ ,

❖ If  $\text{sgn}(f(m_k)) = \text{sgn}(f(a_k))$ , then we let  $a_{k+1} = m_k$  and  $b_{k+1} = b_k$ .

❖ If  $\text{sgn}(f(m_k)) = \text{sgn}(f(b_k))$ , then we let  $a_{k+1} = a_k$  and  $b_{k+1} = m_k$ .


We iterate this over  $\mathbb{N}$  until  $\{f(m_k)\}_{k \geq 1}$  converges to 0.

Now, executing this iteration using an  program, we get that the sequence  $\{f(m_k)\} \rightarrow 0$  as  $\{m_k\} \rightarrow 0.4795832$ . Let us call this number  $p_e$ . Therefore,  $L'(p_e) \approx 0$  and so  $L(p)$  attains either a maxima or a minima at  $p_e$ .

Now, observe that

$$L'(p) = 2p^{45}(1 - p^2)^{76}(23 - 100p^2) = \left[ 2 \cdot \frac{L(p)}{p(1 - p^2)} \right] \cdot (23 - 100p^2)$$

The number inside square brackets is strictly positive when  $p \in (0, 1)$ . So,  $L'(p) \leq 0$  depends on whether  $23 - 100p^2 \leq 0$ . Computation shows that if  $L'(p_e) = 0$  and for  $p \in (0, 1)$ , when  $p < p_e$ ,  $L'(p) > 0$  so  $L$  is increasing. Again, when  $p > p_e$ ,  $L'(p) < 0$  so  $L$  is decreasing. This proves that  $L(p)$  attains its global minima in  $(0, 1)$  at  $p = p_e = 0.4795832$ . Therefore, in the interval  $[0, 1]$ , the  $L$  attains its global maxima at  $p_e$ . So, maximum likelihood estimator of  $p$  is  $p_e$  i.e. 0.4795832.

❖ **Code :** In the  - Script file “**proj-03.r**”, we follow the above-mentioned algorithm. We begin the iterations by setting  $a_0 = 0.2$  and  $b_0 = 0.6$  and stop whenever for some  $k \in \mathbb{N}$ , we get  $f(m_k) < \epsilon$ , where  $\epsilon$  is a pre-defined tolerance value. In the program,  $\epsilon$  has been denoted by “tol” and it’s value is  $10^{-30}$ . Running this program, we get that  $\{m_k\}$  converges to 0.4795832.

❖ **Remark :** This problem can also be solved without any computational numerical methods like Bisection or Newton-Raphson. Since,

$$\begin{aligned} L'(p) = 2p^{45}(1 - p^2)^{76}(23 - 100p^2) = 0 & \iff 23 - 100p^2 = 0 \\ & \iff p = \pm \frac{\sqrt{23}}{10} \approx \pm 0.4795832 \end{aligned}$$

and only  $0.4795832 \in (0, 1)$ , so we can directly say that  $p_e = 0.4795832$  is the maximum likelihood estimator of  $p$ .

## ❖ Project #4

❖ **Answer :**  $L(p, a)$  is maximized when  $p = 1.946419$  and  $a = 2.87889$ .

❖ **Solution :** We are required to maximize the function  $L(p, a)$  w.r.t. both  $p$  and  $a$ , where

$$L(p, a) = \prod_{i=1}^n f(x_i | p, a) = \prod_{i=1}^n \frac{a^p}{\Gamma(p)} \cdot x_i^{p-1} e^{ax_i} = \frac{a^{np}}{[\Gamma(p)]^n} \cdot M^{p-1} e^{aS}$$

where  $n = 996$ ,  $M = \prod_{i=1}^{996} x_i$  and  $S = \sum_{i=1}^{996} x_i$ .

Now,  $L(p, a) > 0$  as  $p > 0$ ,  $a > 0$  and we know that  $\Gamma(p) > 0$  for all  $p > 0$ . So, we can take log on both sides of the preceding expression to obtain

$$\log L(p, a) = np \cdot \log a + (p - 1) \log M - n \cdot \log \Gamma(p) - aS$$

In order for this to attain an extreme value, we need both the partial derivatives of the the function  $L(p, a)$  w.r.t.  $p$  and  $a$  to be equal to 0. Differentiating the last equation accordingly, we obtain

$$g_1(p, a) = \frac{\partial L}{\partial p} = L(p, a) \cdot [n \cdot \log a + \log M - n \cdot \psi(p)]$$

$$g_2(p, a) = \frac{\partial L}{\partial a} = L(p, a) \cdot \left[ \frac{np}{a} - S \right]$$

where  $\psi(p) = \frac{d}{dp} [\log \Gamma(p)] = \frac{\Gamma'(p)}{\Gamma(p)}$  is known to be the Digamma Function.

Now,  $L(p, a)$  attains an extrema when  $g_1(p, a) = g_2(p, a) = 0$ . Since,  $L(p, a) > 0$  for all  $p, a > 0$ , so we have

$$f_1(p, a) = n \cdot \log a + \log M - n \cdot \psi(p) = 0 \quad \& \quad f_2(p, a) = \frac{np}{a} - S = 0$$

From the second-last equation, we get  $\log a = \psi(p) - \frac{1}{n} \log M$ , which implies

$$\begin{aligned} a &= \exp \left[ \psi(p) - \frac{1}{n} \log M \right] \\ &= \exp \left[ \psi(p) + \log M^{-\frac{1}{n}} \right] \\ &= M^{-\frac{1}{n}} e^{\psi(p)} \end{aligned}$$

Substituting this value of  $a$  in the equation  $f_2(p, a) = 0$ , we obtain

$$\frac{S}{n} \cdot M^{-\frac{1}{n}} e^{\psi(p)} = p$$

Now, consider the equation  $\mathcal{H}(p) = \frac{S}{n} \cdot M^{-\frac{1}{n}} e^{\psi(p)} - p$

So, we need to solve for  $p$  such that  $\mathcal{H}(p) = 0$ . In order to do this, we employ **Newton-Raphson iterations** on the sequence  $\{p_k\}_{k \geq 0}$  starting from  $p_0 = 2$ . So, the iteration will look like

$$p_{k+1} = p_k - \frac{\mathcal{H}(p)}{\mathcal{H}'(p)}$$

where

$$\begin{aligned} \mathcal{H}'(p) &= \frac{d\mathcal{H}}{dp} = \frac{d}{dp} \left[ \frac{S}{n} \cdot M^{-\frac{1}{n}} e^{\psi(p)} - p \right] \\ &= \frac{S}{n} \cdot M^{-\frac{1}{n}} e^{\psi(p)} \cdot \psi'(p) - 1 \\ &= \left[ \frac{S}{n} \cdot M^{-\frac{1}{n}} e^{\psi(p)} \cdot \psi'(p) - p + p \right] \cdot \psi'(p) - 1 \\ &= \left[ p + \mathcal{H}(p) \right] \cdot \psi'(p) - 1 \end{aligned}$$

Here,  $\psi'(p)$  is the first derivative of  $\psi(p)$  and it is called the Trigamma Function.


Executing this iteration using an  program, we get that  $\{p_k\}$  converges to  $p_e = 1.946419$  and substituting, we obtain

$$\frac{np_e}{a_e} - S = 0 \iff a_e = \frac{np_e}{S} = 2.87889$$

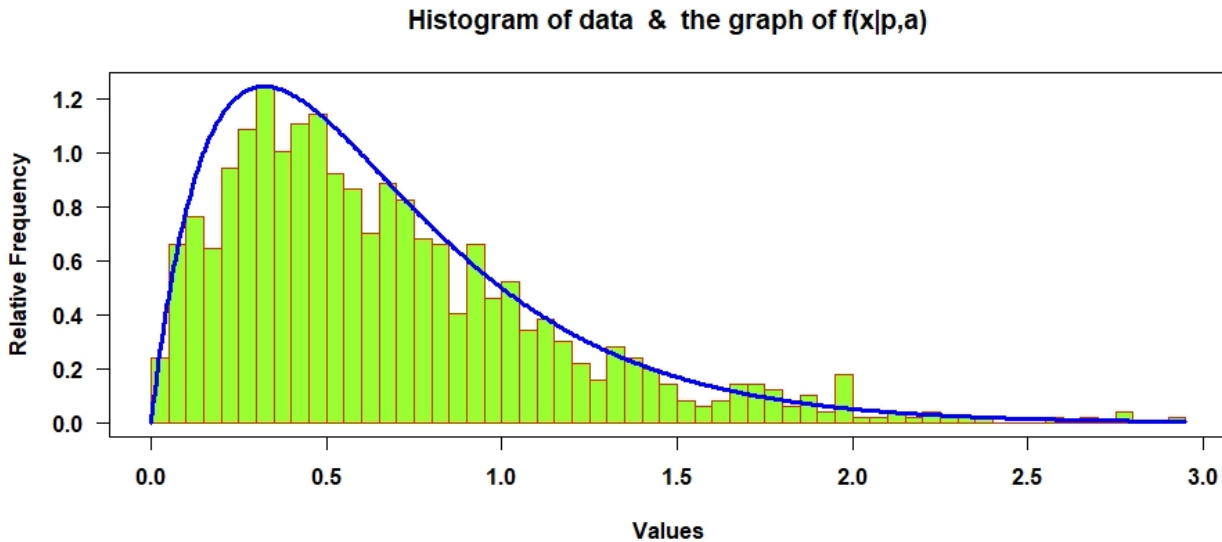
approximately. Let's represent  $(p_e, a_e)$  by  $T$ . Now, observe that

$$\left[ \frac{\partial f_1}{\partial p} \right]_T = -n \cdot \psi'(p_e) = -(0.66727 \times n) < 0 \quad \& \quad \left[ \frac{\partial f_2}{\partial a} \right]_T = -\frac{np_e}{a_e^2} < 0$$

so  $L(p, a)$  is maximized at  $(p_e, a_e)$ . We'll verify this result using a histogram in the last paragraph titled “**Plots**”.

❖ **Code** : In the  - Script file “**proj-04.r**”, we follow the above-mentioned technique and stop the process whenever  $|p_{k+1} - p_k| < \varepsilon$ , where  $\varepsilon$  is a pre-defined tolerance value, very close to 0. In the code, it is represented as “tol” and its value is assigned to be  $1e-8$  or  $10^{-8}$ . Using this method, the Newton-Raphson iterations on  $\mathcal{H}$  produces  $p_e$  and henceforth,  $a_e$ .

❖ **Plots** : Using the observations in the *data.txt* file, we have constructed a histogram below. The contents X-axis and Y-axis are written on the sides of the axes. Now, we superimpose the graph of the function  $f(x | p_e, a_e)$  on the drawn histogram in order to compare their shapes visually. Here is the final diagram :



❖ **Conclusion** : From the above diagram, we can clearly see that the shape of the function  $f$ , when plotted using the numerically computed maximum like-

likelihood estimates of  $p$  and  $a$ , is very similar to the approximate shape described by histogram. This indicates that the fit is good and thus, the computed values of  $p_e$  and  $a_e$  are indeed good approximates. Hence, visually, we may conclude that the maximum likelihood estimates, which we've computed numerically, are correct.

❖ **Remark :** Other than Newton-Raphson iterations, this problem can also be solved using Bisection method. Anyway, even in that procedure, we'll obtain the same  $(p_e, a_e)$  as the maximum likelihood estimators of  $(p, a)$ .

## ❖ Project #6

❖ **Solution :** For given matrices  $\mathbf{A}$  and  $\mathbf{b}$  of orders  $m \times n$  and  $m \times 1$ , we are required to find a least square solution to the system  $\mathbf{Ax} = \mathbf{b}$ , where  $x$  is an  $n$ -dimensional column vector. Mathematically speaking, we need to find an  $n \times 1$  vector  $\mathbf{x}$  among all possible vectors in  $\mathbb{R}^n$  such that  $\|\mathbf{Ax} - \mathbf{b}\|^2$  is minimum.

In order to solve this problem, we employ the **QR Decomposition** of the matrix  $\mathbf{A}$  (If possible), i.e. we write

$$\mathbf{A}_{m \times n} = \mathbf{Q}_{m \times m} \cdot \mathbf{R}_{m \times n}$$

where  $\mathbf{Q}$  is an orthogonal matrix and  $\mathbf{R}$  is an upper triangular matrix. Now, in order to do this, we use the *Householder Transformation*. For each  $i = 1, 2, \dots, n$ , we consider the submatrix  $\mathbf{A}_i = \mathbf{A}[i : m, i : n]$  of  $\mathbf{A}$  and let  $\mathbf{x}_i = (\mathbf{A}_i)_{*1}$  and

$$\mathbf{y}_i = \begin{bmatrix} \|\mathbf{x}_i\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Now, let's define  $\mathbf{u}_i = \text{unit}(\mathbf{x}_i - \mathbf{y}_i)$  and  $\mathbf{H}_i^* = \mathbf{I} - 2\mathbf{u}_i\mathbf{u}_i'$ . For each  $i$ , let

$$\mathbf{H}_i = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_i^* \end{bmatrix}$$

In fact, for finding out a least square solution to a system when  $\mathbf{A}$  is not of full column rank, we might use a technique in which we delete those columns completely which appear to be some linear combination of its preceding columns at some point of pre-multiplication by a Householder matrix. Anyway, in this problem, we haven't used that algorithm.

Instead, in this problem, if at some  $k$ -th step,  $\|\mathbf{u}\| = 0$ , then we let  $\mathbf{H}_k = \mathbf{I}$  and proceed. So, pre-multiplying  $\mathbf{A}$  by  $\mathbf{H}_1, \mathbf{H}_2, \dots, \mathbf{H}_n$  one by one (Shaving method), we get an upper triangular matrix, say  $\mathbf{R}$  with dimension  $m \times n$ . In mathematical notation,

$$(\mathbf{H}_n \mathbf{H}_{n-1} \cdots \mathbf{H}_2 \mathbf{H}_1) \mathbf{A} = \mathbf{R} \iff \mathbf{Q}' \mathbf{A} = \mathbf{R}$$

where  $\mathbf{Q}' = \mathbf{H}_n \mathbf{H}_{n-1} \cdots \mathbf{H}_2 \mathbf{H}_1$  is an orthogonal matrix of dimension  $n \times n$ , since it's the product of  $n$  many orthogonal matrices. Pre-multiplying both sides by  $\mathbf{Q}$ , we get the QR Decomposition of  $\mathbf{A}$ .

- **Fact #1** : Orthogonal transformation (Pre-multiplication by an orthogonal matrix) preserves norm or length, i.e. if  $\mathbf{G}$  is an orthogonal matrix and  $\mathbf{x}$  is a column vector, then  $\|\mathbf{G}\mathbf{x}\| = \|\mathbf{x}\|$ . The proof is following :

$$\|\mathbf{G}\mathbf{x}\| = \sqrt{(\mathbf{G}\mathbf{x})' \cdot \mathbf{G}\mathbf{x}} = \sqrt{\mathbf{x}'(\mathbf{G}'\mathbf{G})\mathbf{x}} = \sqrt{\mathbf{x}'\mathbf{x}} = \|\mathbf{x}\|$$

- **Fact #2** : Since  $\mathbf{Q}$  is orthogonal, so using fact #1, it can be shown that

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 &= \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{Q}\mathbf{R}\mathbf{x} - \mathbf{b}\|^2 \\ &= \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{Q}(\mathbf{R}\mathbf{x} - \mathbf{Q}'\mathbf{b})\|^2 \\ &= \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{R}\mathbf{x} - \mathbf{Q}'\mathbf{b}\|^2 \\ &= \min_{\mathbf{x} \in \mathbb{R}^n} \left[ \|\mathbf{R}_1\mathbf{x} - \mathbf{c}_1\|^2 + \|\mathbf{c}_2\|^2 \right] \\ &= \min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{R}_1\mathbf{x} - \mathbf{c}_1\|^2 + \|\mathbf{c}_2\|^2 \end{aligned}$$

where  $\mathbf{R} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{bmatrix}$ , where  $\mathbf{R}_1$  is an  $n \times n$  upper triangular matrix.


Similarly, we have  $\mathbf{Q}'\mathbf{b} = \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix}$ , where  $\mathbf{c}_1$  is an  $n \times 1$  column vector.



• **Fact #3** : If the matrix  $\mathbf{A}$  is of full column rank, then it has a unique QR Decomposition. Moreover, in that case, the least square solution will be unique too. Also, we have,

$$\rho(\mathbf{R}_1) = \rho \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{0} \end{bmatrix} = \rho \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{bmatrix} = \rho(\mathbf{R}) = \rho(\mathbf{Q}'\mathbf{A}) = \rho(\mathbf{A}) = n$$

implying that  $\mathbf{R}_1$  is of full column rank and hence, non-singular. In that case,  $\mathbf{R}_1\mathbf{x} = \mathbf{c}_1$  is a consistent system, i.e.  $\exists \mathbf{x}$  such that  $\|\mathbf{R}_1\mathbf{x} - \mathbf{c}_1\|^2 = 0$ . This  $\mathbf{x}$  is the unique least square solution to our original system  $\mathbf{Ax} = \mathbf{b}$ . In case  $\rho(\mathbf{A}) < n$ , then  $\mathbf{R}_1\mathbf{x} = \mathbf{c}_1$  is either inconsistent, or it has infinitely many solutions. Even there, we can find a least square solution, but in our problem, those cases are mostly ignored.

❖ **Code** : In the  - Script file “**proj-06.r**”, we follow the above-mentioned technique, but in a more efficient way. In each step of Householder Transformation, we compute  $\mathbf{u}$  and carry out the pre-multiplication of  $\mathbf{H}_i$  with each columns of the latest updated  $\mathbf{A}$  matrix in the following way :

$$\begin{aligned} \mathbf{H}_i\mathbf{x} &= (\mathbf{I} - 2\mathbf{u}_i\mathbf{u}_i') \cdot \mathbf{x} \\ &= \mathbf{x} - 2\mathbf{u}_i \cdot (\mathbf{u}_i'\mathbf{x}) \\ &= \mathbf{x} - \underbrace{(2\mathbf{u}_i'\mathbf{x}) \cdot \mathbf{u}_i}_{(2n+1) \text{ multiplications}} \end{aligned}$$

This is possible since  $\mathbf{u}_i'\mathbf{x}$  is a scalar. In the above process, the number of multiplications for each column reduces to  $(2n + 1)$  instead of  $n^2$ , thus computationally efficient.

Now, after shaving a column, we overwrite  $\mathbf{u}_i$  it on the shaved portion of the corresponding column (Lower triangular portion of  $\mathbf{A}$ ). The topmost numbers of the corresponding columns in all the steps are stored separately in a vector  $D$ . So, the final content of  $D$  is basically the principal diagonal elements of  $\mathbf{R}_1$ . Rest of the  $\mathbf{R}_1$  matrix is overwritten on the upper triangular portion of  $\mathbf{A}$ . So, the final product of this operation is an updated (overwritten) matrix  $\mathbf{A}$ , hence a very little extra memory is required to store the  $\mathbf{R}_1$  and the  $\mathbf{u}_i$ 's. So, on a whole, **this implementation is very efficient.**

After updating  $\mathbf{A}$ , we use the efficiently stored  $\mathbf{R}_1$  matrix, we compute the required least square solution by backward substitution. If  $\mathbf{A}$  has rank  $\leq n$ , we check if there are infinitely many solutions to the system  $\mathbf{R}_1 \mathbf{x} = \mathbf{c}_1$  and if so, we show any one possible solution as the least square solution. If  $\mathbf{R}_1 \mathbf{x} = \mathbf{c}_1$  is inconsistent, we print "ERROR: Given matrix is not of full column rank!". Our program gives the efficiently computed QR matrix, the principal diagonal elements of  $\mathbf{R}$  and a least square solution as its output.

## \* Project #7

❖ **Notations :** All the notations used in our solution are either standard, or described in our class web-page. For example, the  $k$ th order divided difference of  $f$  is denoted by  $f[x_k, \dots, x_0]$ .

❖ **Solution :** Suppose, we are given  $(n + 1)$  many points on the real plane, viz.  $A_0 \equiv (x_0, y_0), A_1 \equiv (x_1, y_1), \dots, A_n \equiv (x_n, y_n)$ . We are required to show that if we traverse through the divided difference table made on the basis of these points and construct a polynomial accordingly, we'll end up getting the same polynomial as the forward interpolating polynomial. We'll use Newton divided difference formula, two observations and a lemma to prove this.

• **Newton's divided difference formula :** For any  $(n+1)$  many given points say  $(p_1, q_1), (p_2, q_2), \dots, (p_n, q_n)$ , there exists a unique interpolating polynomial  $h$  (depending on those points) with  $\deg(h) \leq n$ , such that  $h(p_i) = q_i$  for  $i = 0(1)n$ . The expression of  $h$  looks like

$$\begin{aligned} h(p) = & h[p_0] + \\ & (p - p_0) \cdot h[p_1, p_0] + \\ & (p - p_0)(p - p_1) \cdot h[p_2, p_1, p_0] + \\ & (p - p_0)(p - p_1)(p - p_2) \cdot h[p_3, p_2, p_1, p_0] + \dots + \\ & (p - p_0) \cdots (p - p_{n-1}) \cdot h[p_n, \dots, p_0] \end{aligned}$$

By this formula, for our  $A_0, A_1, \dots, A_n$ , there is a polynomial, say  $f$ , with  $\deg(f) \leq n$  which interpolates these points.

- **Lemma ( $\mathbb{M}$ )** : The interpolating polynomial of degree  $\leq n$ , mentioned above, is unique for the given set of  $(n + 1)$  points.

Now, let us construct the polynomial as instructed in the problem statement. We define  $z_i$ 's in the following way :

- ✱ Suppose, we begin our traversal from  $y_k$  for some integer  $k \in [0, n]$ . Then, we define its corresponding  $x_k$  to be  $z_0$ . Obverse that the shadow of  $f[x_k]$  is  $\{x_k\}$  or  $\{z_0\}$ .
- ✱ In the 1st step, we may move to  $f[x_k, x_{k-1}]$  or  $f[x_{k+1}, x_k]$ . Suppose, without loss of generality, we move to  $f[x_{k+1}, x_k]$ . Then, we define  $z_1$  to be the newly included point, i.e.  $x_{k+1}$ . Observe that the shadow of  $f[x_{k+1}, x_k]$  is  $\{x_{k+1}, x_k\}$  or  $\{z_1, z_0\}$ .
- ✱ In the 2nd step, we may move to  $f[x_{k+1}, x_k, x_{k-1}]$  or  $f[x_{k+2}, x_{k+1}, x_k]$ . Suppose, w.l.o.g., we move to  $f[x_{k+1}, x_k, x_{k-1}]$ . Then, we define  $z_2$  to be the newly included point, i.e.  $x_{k-1}$ . Observe that the shadow of  $f[x_{k+1}, x_k, x_{k-1}]$  is  $\{x_{k+1}, x_k, x_{k-1}\}$  or  $\{z_2, z_1, z_0\}$ .
- ✱ In general, we define  $z_i$  to be the new  $x_j$  which is reached after the  $i$ th step in the traversal. So, the shadow of  $f[z_i, \dots, z_0]$  is basically  $\{z_i, \dots, z_0\}$ .
- ✱ Proceeding in this similar manner, after  $n$  steps, we'll reach  $f[x_n, \dots, x_1, x_0]$  eventually. So, clearly the shadow of  $f[x_n, \dots, x_1, x_0]$  will be  $\{z_n, \dots, z_1, z_0\}$ .

Summing up this whole process, we get that by this traversal via an arbitrary path as per the instructions of the problem, we obtain a polynomial (Say  $g$ ), which looks like

$$\begin{aligned} g(x) = & f[z_0] + \\ & (x - z_0) \cdot h[z_1, z_0] + \\ & (x - z_0)(x - z_1) \cdot h[z_2, z_1, z_0] + \\ & (x - z_0)(x - z_1)(x - z_2) \cdot h[z_3, z_2, z_1, z_0] + \dots + \\ & (x - z_0) \cdots (x - z_{n-1}) \cdot h[z_n, \dots, z_0] \end{aligned}$$

- **Observation ( $\star$ )** : In the traversal process, we start from some  $f[x_k]$  and name it as  $z_0$  and after  $n$  steps, finally we reach  $f[x_n, \dots, x_1, x_0]$ . So, right after

beginning, we cover one  $x_i$  and at each of the next  $n$  steps, a new  $x_i$  is included. Since the total number of possible  $x_i$  is exactly  $(n + 1)$ , so this proves that all  $x_i$ 's are exhausted in the last step. **Therefore,  $\{z_0, z_1, \dots, z_n\}$  is actually a permutation of  $\{x_0, x_1, \dots, x_n\}$ .**

We consider the points  $B_0 \equiv (z_0, f(z_0))$ ,  $B_1 \equiv (z_1, f(z_1))$ ,  $\dots$ ,  $B_n \equiv (z_n, f(z_n))$  which, by **Observation (★)**, is just a permutation of the points  $A_0, A_1, A_2, \dots, A_n$ .

We construct a divided difference table on the basis of  $B_0, B_1, \dots, B_n$  and traverse through the forward path.

$z_0$	$f[z_0]$				
		$f[z_1, z_0]$			
$z_1$	$f[z_1]$		$f[z_2, z_1, z_0]$		
		$f[z_2, z_1]$		$\dots$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$f[z_{n-1}, z_{n-2}, \dots, z_0]$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\dots$	$f[z_n, z_{n-1}, \dots, z_1, z_0]$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		$f[z_n, z_{n-1}, \dots, z_1]$
		$f[z_{n-1}, z_{n-2}]$		$\dots$	
$z_{n-1}$	$f[z_{n-1}]$		$f[z_n, z_{n-1}, z_{n-2}]$		
		$f[z_n, z_{n-1}]$			
$z_n$	$f[z_n]$				

- **Observation (✚)** : From the above divided difference table and applying Newton's Divided Difference Formula, we obtain that the polynomial of degree  $\leq n$  which interpolates the points  $B_0, B_1, \dots, B_n$  will be

$$\begin{aligned}
 & f[z_0] + \\
 & (z - z_0) \cdot h[z_1, z_0] + \\
 & (z - z_0)(z - z_1) \cdot h[z_2, z_1, z_0] + \\
 & (z - z_0)(z - z_1)(z - z_2) \cdot h[z_3, z_2, z_1, z_0] + \dots + \\
 & (z - z_0) \dots (z - z_{n-1}) \cdot h[z_n, \dots, z_0]
 \end{aligned}$$

which is precisely the expression of  $g(z)$ . This proves that  $g$  is the unique interpolating polynomial which interpolates  $B_0, B_1, \dots, B_n$ .

Now, we summarize what we have got. Here's the comparison between the interpolating polynomials  $f$  and  $g$  :

- ✱ Both  $f$  and  $g$  are real polynomials with  $\deg(f) \leq n$  and  $\deg(g) \leq n$ .
- ✱  $f$  interpolates the set of points  $\{A_0, \dots, A_n\}$  and  $g$  interpolates the set of points  $\{B_0, \dots, B_n\}$  which is a permutation of  $\{A_0, \dots, A_n\}$ . So, both  $f$  and  $g$  basically interpolates the same set of  $(n + 1)$  points.

But, by **Lemma (M)**, we know that such an interpolating polynomial is unique !

Therefore,  $f \equiv g$

Since our chosen path in the beginning of the proof was completely arbitrary, so the result that  $f \equiv g$  holds for all such permitted paths. Therefore, whatever valid path we choose, we'll always end up getting the unique interpolating polynomial. **[Proved]**  $\square$

❖ **Visual Representation :** In the file “**proj-07.pptx**”, there is a rough demonstration of the above-mentioned procedure for the case  $n = 5$ . Since the writing of the solution is somewhat tedious, so a visual representation may help it being a little more clear.

## ✱ Project #9

❖ **Solution :** Crout's decomposition is a special case of LU decomposition of a non-singular matrix, where all the elements in the principal diagonal of  $U$  is taken to be equal to 1. In general, LU decomposition is not unique, but it can be shown that Crout's decomposition for a matrix is always unique (if exists).

At first, we may assume that  $A$  is non-singular. In that case, if we are interested in finding out the solution to the equation  $Ax = b$ , then we proceed like:

$$Ax = b \implies LUx = b \implies Ly = b$$

This system is easily solvable using forward substitution. So, if  $y_0$  is the solution, then we get  $Ux = y_0$  which can be solved by backward substitution.

Now, for a square matrix  $\mathbf{A}$  of order  $n$ , if its LU decomposition exists, then we consider its unique Crout's decomposition. For the matrix  $\mathbf{U}$ , we have  $u_{ii} = 1$  for all  $i = 1(1)n$ . It can be easily shown that

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik}u_{kj} \quad \text{when } i \geq j$$

$$u_{ij} = \frac{1}{l_{ii}} \left[ a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj} \right] \quad \text{when } i < j$$

The above is true only if  $l_{ii} \neq 0$  for each  $i$ . Otherwise, for some  $i$ , if both the numerator and denominator of the last equation are equal to 0, then Crout's decomposition exists, but it will not be unique. For  $i < j$ , the actual form of the second equation is

$$l_{ii}u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj} = D_{ij}$$


Now, there are 3 possible cases, which determine whether the system has a unique solution or infinitely many solutions or the system is inconsistent.

- **Case #1** : If  $D_{ij} \neq 0$  and  $l_{ii} \neq 0$ , then  $u_{ij}$  may take any real value. Then, the decomposition is clearly not unique.
- **Case #2** : If  $D_{ij} = 0$  and  $l_{ii} \neq 0$ , then  $u_{ij}$  must be 0. In that case, its value is unique.
- **Case #3** : If  $D_{ij} = 0$  and  $l_{ii} = 0$ , then no real value of  $u_{ij}$  satisfies the equation. In that case, there won't exist any such decomposition.

Once we obtain a possible LU decomposition (not necessarily unique), at first we are required to solve the system  $\mathbf{Ly} = \mathbf{b}$  using forward substitution. Exactly similarly as before, there will be 3 cases and clearly, any solution won't exist if for some  $i$ ,

$$l_{ii} = 0 \quad \text{and} \quad b_i - \sum_{k=1}^{i-1} l_{ik}x_k \neq 0$$

Otherwise, they're will be at least one solution (Say  $\mathbf{y}_0$ ) to the system. Since, all the principal diagonal elements of  $\mathbf{U}$  are 1, so its determinant is 1, so  $\mathbf{U}$  is non-singular. Therefore, there will be a solution (Say  $\mathbf{x}_0$ ) to the original system, whose uniqueness depends on the uniqueness of the LU decomposition of  $\mathbf{A}$ .

❖ **Code :** In the  - Script file “**proj-09.r**”, we follow the above-mentioned technique in an efficient manner.

We already know that the principal diagonal elements of  $\mathbf{U}$  are all 1. Also, interestingly,  $\mathbf{L}$  and  $\mathbf{U}$  have nonzero elements at different positions. This ensures that we can somehow manage to store the matrices  $\mathbf{L}$  and  $\mathbf{U}$  in place of  $\mathbf{A}$ . Observe that for  $i < j$ , the value of  $a_{ij}$  is required to compute  $l_{ij}$  only. Similarly, for  $i \geq j$ , the value of  $a_{ij}$  is required to compute  $u_{ij}$  only. Thus, after the end of computation of such  $l_{ij}$  and  $u_{ij}$  in each step, we can simply overwrite them in place of  $a_{ij}$ . Therefore, no extra memory (storage) will be used for storing the matrices  $\mathbf{L}$  and  $\mathbf{U}$ . Therefore, **this method is computationally efficient.**

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