

# MA 214: Numerical Analysis Notes

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Until: Lecture 12

## DISCLAIMER

This is just a collection of formulae/algorithms compiled together.

In the case of algorithms, I explain the procedure concisely. However, do not take this as a substitute for lecture slides as I don't go into the theory at all.

Also, I've modified some things compared to the lecture slides wherever I felt it was an error. So, be warned. Sometimes, I also change the order in the notes compared to how it was taught in slides if I feel like that's more efficient.

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## 1 Interpolation

### 1. Lagrange Polynomials

Let  $x_0, x_1, \dots, x_n$  be  $n+1$  distinct points in  $[a, b]$ . Let  $f : [a, b] \rightarrow \mathbb{R}$  be a function whose value is known at those aforementioned points.

We want to construct a polynomial  $p(x)$  of degree  $\leq n$  such that  $p(x_i) = f(x_i)$  for all  $i \in \{0, \dots, n\}$ .

Towards this end, we define the polynomials  $I_k(x)$  for  $k \in \{0, \dots, n\}$  in the following manner:

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

(Intuitive understanding:  $I_k$  is a degree  $n$  polynomial such that  $I_k(x_j) = 0$  if  $k \neq j$  and  $I_k(x_k) = 1$ .)

Now, define  $p(x)$  as follows:

$$p(x) := \sum_{i=0}^n f(x_i) I_i(x)$$

### 2. Newton's form

Let  $x_0, x_1, \dots, x_n$  be  $n+1$  distinct points in  $[a, b]$ . Let  $f : [a, b] \rightarrow \mathbb{R}$  be a function whose value is known at those aforementioned points.

We want to construct a polynomial  $P_n(x)$  of degree  $\leq n$  such that  $p(x_i) = f(x_i)$  for all  $i \in \{0, \dots, n\}$ .

We define the divided differences (recursively) as follows:

$$\begin{aligned} f[x_0] &:= f(x_0) \\ f[x_0, x_1, \dots, x_k] &:= \frac{f[x_1, \dots, x_k] - f[x_0, \dots, x_{k-1}]}{x_k - x_0} \end{aligned} \quad \text{for all } 1 < k \leq n$$

With this in place, the desired polynomial  $P_n(x)$  is (not so) simply:

$$\begin{aligned} P_n(x) &:= f[x_0] + f[x_0, x_1](x - x_0) \\ &\quad + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &\quad + \dots \\ &\quad \vdots \\ &\quad + f[x_0, x_1, \dots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1}) \end{aligned}$$

*Remarks.* Note that  $x - x_n$  does not appear in the last term.

Note that given  $P_n(x)$ , it is simple to construct  $P_{n+1}(x)$ .

### 3. Osculatory Interpolation

This is essentially the same as the previous case.

I'll state the problem in the form I think is the simplest. (Any other form can be reduced to this.)

Suppose we are given  $k + 1$  distinct points  $x_0, \dots, x_k$  in  $[a, b]$  and a function  $f : [a, b] \rightarrow \mathbb{R}$  which is sufficiently differentiable.

Suppose we are given the following values:

$$\begin{aligned} &f^{(0)}(x_0), f^{(1)}(x_0), \dots, f^{(m_1-1)}(x_0) \\ &f^{(0)}(x_1), f^{(1)}(x_1), \dots, f^{(m_2-1)}(x_1) \\ &\vdots \\ &f^{(0)}(x_k), f^{(1)}(x_k), \dots, f^{(m_k-1)}(x_k) \end{aligned}$$

(Notation:  $f^{(0)}(x) = f(x)$  and  $f^{(n)}(x)$  is the  $n^{\text{th}}$  derivative.)

Thus, we are given  $m_1 + m_2 + \dots + m_k =: n + 1$  data. As usual, we now want to compute a polynomial  $P_n(x)$  that agrees with  $f$  at all the data. (That is, all the given derivatives must also be same.) As it goes without saying,  $P_n(x)$  must have degree  $\leq n$ .

To do this, we list the above points as follows:

$$\underbrace{x_0, x_0, \dots, x_0}_{m_1}, \underbrace{x_1, x_1, \dots, x_1}_{m_2}, \dots, \underbrace{x_k, x_k, \dots, x_k}_{m_k}.$$

Now, we just apply the above (Newton's) formula with the following modification in the definition of the divided difference:

$$f[\underbrace{x_i, x_i, \dots, x_i}_{p+1 \text{ times}}] := \frac{f^{(p)}(x_i)}{p!}.$$

### 4. Richardson Extrapolation

Suppose that for sufficiently small  $h \neq 0$ , we have the formula:

$$M = N_1(h) + k_1 h + k_2 h^2 + k_3 h^3 + \dots,$$

for some constants  $k_1, k_2, k_3, \dots$ .

Define the following:

$$N_j(h) := N_{j-1}(h/2) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1} \quad \text{for } j \geq 2.$$

Choose some  $h$  *sufficiently small* (whatever that means). Then,  $N_j(h)$  keeps becoming a better approximation of  $M$  as  $j$  increases.

We create a table of  $h$  and  $N_j(h)$  as follows:

$h$	$N_1(h)$	$N_2(h)$	$N_3(h)$	$N_4(h)$
$h$	$N_1(h)$			
$h/2$	$N_1(h/2)$	$N_2(h)$		
$h/4$	$N_1(h/4)$	$N_2(h/2)$	$N_3(h)$	
$h/8$	$N_1(h/8)$	$N_2(h/4)$	$N_3(h/2)$	$N_4(h)$

$N_4(h)$  will be a good approximation, then.

(Look at slide 15 of Lecture 7 for an example.)

#### Special case

Sometimes, we may have the following scenario:

$$M = N_1(h) + k_2 h^2 + k_4 h^4 + \dots.$$

In this case, we define:

$$N_j(h) := N_{j-1}(h/2) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1} \quad \text{for } j \geq 2.$$

Then, we do the remaining stuff as before.

## 2 Numerical Integration

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

### 1. Rectangle Rule

$$I \approx (b-a)f(a)$$

$$E^R = f'(\eta) \frac{(b-a)^2}{2}, \text{ for some } \eta \in [a, b]$$

### 2. Midpoint Rule

$$I \approx (b-a)f\left(\frac{a+b}{2}\right)$$

$$E^M = \frac{f''(\eta)}{24}(b-a)^3, \text{ for some } \eta \in [a, b]$$

### 3. Trapezoidal Rule

$$I \approx \frac{1}{2}(b-a)[f(a) + f(b)]$$

$$E^T = -f''(\eta) \frac{(b-a)^3}{12}, \text{ for some } \eta \in [a, b]$$

### 4. Corrected Trapezoidal

$$I \approx \frac{1}{2}(b-a)[f(a) + f(b)] + \frac{(b-a)^2}{12}(f'(a) - f'(b))$$

$$E^{CT} = f^{(4)}(\eta) \frac{(b-a)^5}{720}, \text{ for some } \eta \in [a, b]$$

### 5. Composite Trapezoidal

$$I \approx \frac{h}{2} \left[ f(x_0) + 2 \sum_{i=1}^{N-1} f(x_i) + f(x_N) \right]$$

$$E_C^T = -f''(\xi) \frac{h^2(b-a)}{12}, \text{ for some } \xi \in [a, b]$$

Here,  $Nh = b - a$  and  $x_i = a + ih$ .

### 6. Simpson's Rule

$$I \approx \frac{b-a}{6} \left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right\}$$

$$E^S = -\frac{1}{90}f^{(4)}(\eta) \left(\frac{b-a}{2}\right)^5, \text{ for some } \eta \in [a, b]$$

### 7. Composite Simpson's

$$I \approx \frac{h}{6} \left[ f(x_0) + 2 \sum_{i=1}^{N-1} f(x_i) + 4 \sum_{i=1}^N f\left(x_{i-1} + \frac{h}{2}\right) + f(x_N) \right]$$

$$E_C^S = -f^{(4)}(\xi) \frac{(h/2)^4(b-a)}{180}, \text{ for some } \xi \in [a, b]$$

Here,  $Nh = b - a$  and  $x_i = a + ih$ .

## 8. Gaussian Quadrature

Let  $Q_{n+1}(x)$  denote the  $(n+1)^{\text{th}}$  Legendre polynomial.

Let  $r_0, \dots, r_{n+1}$  be its roots. (These will be distinct, symmetric about the origin and will lie in the interval  $[-1, 1]$ .)

For each  $i \in \{0, \dots, n\}$ , we define  $c_i$  as follows:

$$c_i := \int_{-1}^1 \left( \prod_{k=0, k \neq i}^n \frac{x - x_k}{x_i - x_k} \right) dx.$$

Then, we have

$$\int_{-1}^1 f(x) dx \approx \sum_{i=0}^n f(r_i) c_i.$$

Moreover, if  $f$  is a polynomial of degree  $\leq 2n+1$ , then the above is “approximation” is exact.

Standard values:

$n = 0$  :  $Q_1(x) = x$  and  $x_0 = 0$ .  $c_0 = 2$ .

$n = 1$  :  $Q_2(x) = x^2 - \frac{1}{3}$  and  $x_0 = -\frac{1}{\sqrt{3}}$ ,  $x_1 = \frac{1}{\sqrt{3}}$ .  $c_0 = c_1 = 1$ .

$n = 2$  :  $Q_3(x) = x^3 - \frac{3}{5}x$  and  $x_0 = -\sqrt{\frac{3}{5}}$ ,  $x_1 = 0$ ,  $x_2 = \sqrt{\frac{3}{5}}$ .  $c_0 = c_2 = 5/9$ ,  $c_1 = 8/9$ .

## 9. Improper integrals using Taylor series method

Suppose we have  $f(x) = \frac{g(x)}{(x-a)^p}$  for some  $0 < p < 1$  and are asked to calculate  $I = \int_a^b f(x) dx$ .

For the sake of simplicity, I assume  $a = 0$  and  $b = 1$ .

Let  $P_4(x)$  denote the fourth Taylor polynomial of  $g$  around  $a$ . (In this case 0.)

Now, compute  $I_1 = \int_0^1 \frac{P_4(x)}{x^p} dx$ . This can be integrated exactly. (Why?)

Now, we approximate  $I - I_1$ .

Define

$$G(x) := \begin{cases} \frac{g(x) - P_4(x)}{x^p} & \text{if } 0 < x \leq 1 \\ 0 & \text{if } x = 0 \end{cases}$$

Then, approximate  $I_2 = \int_0^1 G(x) dx$  using the composite Simpson's rule.

Then,  $I = I_1 + I_2$ .

For the case of  $a = 0$ ,  $b = 1$  and  $N = 2$  for the composite Simpson's part, we get that  $I_2 \approx \frac{1}{12}[2G(0.5) + 4G(0.25) + 4G(0.75) + G(1)]$ .

That is, finally:

$$I \approx \int_0^1 \frac{P_4(x)}{x^p} dx + \frac{1}{12}[2G(0.5) + 4G(0.25) + 4G(0.75) + G(1)].$$

## 10. Adaptive Quadrature

Let  $I = \int_a^b f(x) dx$  be the integral that we want to approximate.

Suppose that  $\epsilon$  is the accuracy to which we want  $I$ . That is, we want a number  $P$  such that  $|P - I| < \epsilon$ .

Here is what you do:

Subdivide  $[a, b]$  into  $N$  intervals:  $[x_0, x_1]$ ,  $[x_1, x_2]$ ,  $\dots$ ,  $[x_{n-1}, x_n]$ . (Naturally,  $a = x_0 \leq x_1 \leq \dots \leq x_n = b$ .)

Now, for each subinterval, compute the following values:

$$S_i = \frac{h}{6} \left( f(x_i) + 4f\left(x_i + \frac{h}{2}\right) + f(x_{i+1}) \right), \text{ and}$$

$$\overline{S}_i = \frac{h}{12} \left( f(x_i) + 4f\left(x_i + \frac{h}{2}\right) + 2f\left(x_i + \frac{h}{2}\right) + 4f\left(x_i + \frac{3h}{4}\right) + f(x_{i+1}) \right).$$

Now, calculate  $E_i = \frac{1}{15}|\overline{S}_i - S_i|$ .

Now, if  $E_i \leq \frac{x_i - x_{i-1}}{b-a} \epsilon$ , then move on to the next interval.

Otherwise, subdivide again to better approximate  $\int_{x_{i-1}}^{x_i} f(x)dx$ .

Finally, sum up all the  $\overline{S_i}$ s and that's the answer. That is,

$$I \approx P = \sum_{i=1}^n \overline{S_i}.$$

### 11. Romberg Integration

Essentially the baby of composite Trapezoidal rule and Romberg integration.

Suppose we want to calculate  $\int_a^b f(x)dx$ .

Let  $N$  be a power of 2.

$$T_N := \frac{h}{2} \left[ f(x_0) + 2 \sum_{i=1}^{N-1} f(a + ih) + f(x_N) \right], \text{ where } Nh = b - a.$$

Note that  $T_N$  can be computed using  $T_{N/2}$  (assuming  $N \neq 2^0$ ) as:

$$T_N = \frac{T_{N/2}}{2} + h \sum_{i=1}^{N/2} f(a + (2i-1)h).$$

Now for  $m \geq 1$ , we define:

$$T_N^m = T_N^{m-1} + \frac{T_N^{m-1} - T_{N/2}^{m-1}}{4^m - 1}.$$

(Where  $T_N^0$  is just  $T_N$ .)

(Also, for some reason,  $T'_N$  has been used instead of  $T_N^1$ .)

Note that  $\frac{N}{2^m}$  must be an integer for  $T_N^m$  to be defined. We create a table as follows:

$N$	$T_N$	$T'_N$	$T_N^2$	$T_N^3$
1	$T_1$			
2	$T_2$	$T_2^1$		
4	$T_4$	$T_4^1$	$T_4^2$	
8	$T_8$	$T_8^1$	$T_8^2$	$T_8^3$

$T_8^3$  will be a good approximation, then.

(Look at slide 25 of Lecture 7 for an example.)

*Remark.* It can be shown that  $I = T_N + c_2 h^2 + c_4 h^4 + \dots$ . This is why we used the special case formula of 1. 4.

## 3 Numerical Differentiation

1.

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}$$

$$E(f) = -\frac{1}{2} h f''(\eta) \quad \text{for some } \eta \in [a, a+h].$$

2. Central Difference Formula

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h}$$

$$E(f) = -\frac{1}{6} h^3 f^{(3)}(\eta) \quad \text{for some } \eta \in [a-h, a+h].$$

Note that this is an  $O(h^2)$  approximation. Thus, we can use the special case of §1. 4. for better accuracy.

3.

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}$$

$$E(f) = \frac{1}{3} h^3 f^{(3)}(\eta) \quad \text{for some } \eta \in [a, a+2h].$$

Formula 2 is always the better one whenever applicable. At end points, formula 3 is better than formula 1.

#### 4. Central difference for second derivative

$$f''(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi),$$

for some  $\xi \in (x_0 - h, x_0 + h)$ .

#### 5. Solving boundary-value problems in ODE

Suppose that we want to solve the following (linear) ODE:

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

in the interval  $[a, b]$  such that we know  $y(a) = \alpha$ , and  $y(b) = \beta$ .

Set  $h := \frac{b-a}{N}$  for some  $N \in \mathbb{N}$  and  $x_0 = a + ih$  for  $h \in \{0, 1, \dots, N\}$ .

Using central difference approximation, we set up  $N - 1$  linear equations as follows:

$$\begin{aligned} \frac{y_{i-1} - 2y_0 + y_i}{h^2} + f(x_i)\frac{y_{i+1} - y_{i-1}}{2h} + g(x_i)(y_i) &= q(x_i) \\ i &= 1, 2, \dots, N - 1 \end{aligned}$$

The above equations can be rearranged as:

$$\left(1 - \frac{hf_i}{2}\right)y_{i-1} + (-2 + h^2g_i)y_i + \left(1 + \frac{hf_i}{2}\right)y_{i+1} = h^2q_i,$$

for  $i = 1, \dots, N - 1$ ; where  $f_i = f(x_i)$  and so on.

## 4 Solution of non-linear equations

Let  $f$  be a continuous function on  $[a_0, b_0]$  such that  $f(a_0)f(b_0) < 0$  in all these cases. We want to find a root of  $f$  in  $[a_0, b_0]$ . (Existence is implied.)

#### 1. Bisection Method

Set  $n = 0$  to start with.

Loop over the following:

Set  $m = \frac{a_n + b_n}{2}$ .

If  $f(a_n)f(m) < 0$ , then set  $a_{n+1} = a_n$  and  $b_{n+1} = m$ .

Else, set  $a_{n+1} = m$  and  $b_{n+1} = b_n$ .

Increase  $n$  by one.

We still have a root in  $[a_n, b_n]$ .

#### 2. Regula-falsi or false-position method

Set  $n = 0$  to start with.

Loop over the following:

Set  $w = \frac{f(b_n)a_n - f(a_n)b_n}{f(b_n) - f(a_n)}$ .

If  $f(a_n)f(w) < 0$ , then set  $a_{n+1} = a_n$  and  $b_{n+1} = w$ .

Else, set  $a_{n+1} = w$  and  $b_{n+1} = b_n$ .

Increase  $n$  by one.

We still have a root in  $[a_n, b_n]$ .

#### 3. Modified regula-falsi

Set  $n = 0$  and  $w_0 = a_0$  to start with.

Loop over the following:

Set  $F = f(a_n)$  and  $G = f(b_n)$ .

Set  $w_{n+1} = \frac{Ga_n - Fb_n}{G - F}$ .

If  $f(a_n)f(w_{n+1}) \leq 0$ , then set  $a_{n+1} = a_n$  and  $b_{n+1} = w_{n+1}$  and  $G = f(w_{n+1})$ .  
 Furthermore, if we also have  $f(w_n)f(w_{n+1}) > 0$ , set  $F = \frac{F}{2}$ .  
 Else, set  $a_{n+1} = w_{n+1}$  and  $b_{n+1} = b_n$  and  $F = f(w_{n+1})$ .  
 Furthermore, if we also have  $f(w_n)f(w_{n+1}) > 0$ , set  $G = \frac{G}{2}$ .  
 Increase  $n$  by one.  
 We still have a root in  $[a_n, b_n]$ .

#### 4. Secant method

Set  $x_0 = a$ ,  $x_1 = b$  and until satisfied, keep computing  $x_n$  given by

$$x_{n+1} = \frac{f(x_n)x_{n-1} - f(x_{n-1})x_n}{f(x_n) - f(x_{n-1})} \quad \text{for } n \geq 1.$$

*Remark.* This process will be forced to stop if we arrive at  $f(x_n) = f(x_{n-1})$  at some point.

## 5 Iterative methods

### 1. Newton's Method

You are given a function  $f$  which is continuously differentiable and you want to find its root. You are also given some  $x_0$ .

Compute the following sequence recursively until satisfied:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{for } n \geq 0.$$

### 2. Fixed point iteration

Let  $I$  be a closed interval in  $\mathbb{R}$ . Let  $f : I \rightarrow I$  be a differentiable function such that there exists some  $K \in [0, 1)$  such that  $|f'(x)| \leq K$  for all  $x \in I$ .

Then, there is a unique  $\xi \in I$  such that  $f(\xi) = \xi$ . To find this fixed point, choose any  $x_0 \in I$  and define the sequence

$$x_n := f(x_{n-1}) \quad n \geq 1.$$

Then,  $x_n \rightarrow \xi$ .

### 3. Aitken's $\Delta^2$ Process

**Definition.** Given a sequence  $(x_n)$ , let  $\Delta x_n := x_{n+1} - x_n$ .

Then,  $\Delta^2 x_n = x_{n+2} - 2x_{n+1} + x_n$ .

Given a sequence  $x_0, x_1, \dots$  converging to  $\xi$ , calculate  $\widehat{x_1}, \widehat{x_2}, \dots$  by

$$\widehat{x_n} := x_{n+1} - \frac{(\Delta x_n)^2}{\Delta^2 x_{n-1}}.$$

Then,  $\widehat{x_n} \rightarrow \xi$ .

If the sequence  $x_0, x_1, \dots$  converges linearly to  $\xi$ , that is, if

$$\xi - x_{n+1} = K(\xi - x_n) + \theta(\xi - x_n), \quad \text{for some } K \neq 0$$

then  $\widehat{x_n} = \xi + O(\xi - x_n)$ , that is,  $\frac{\widehat{x_n} - \xi}{x_n - \xi} \rightarrow 0$ .

### 4. Steffensen iteration

Let  $g(x)$  be the function whose fixed point is desired. Let  $y_0$  be some given point.

Set  $n = 0$  to start with.

Loop over the following:

Set  $x_0 = y_n$ .

Set  $x_1 = g(x_0)$ ,  $x_2 = g(x_1)$ .

Set  $\Delta x_1$  and  $\Delta^2 x_0$ .

Set  $y_{n+1} = x_2 - \frac{(\Delta x_1)^2}{\Delta^2 x_0}$ .

Increase  $n$  by 1.

Note that we get a sequence  $y_0, y_1, y_2, \dots$ . However, we only ever have  $x_0, x_1$  and  $x_2$ .

**Definition 1.** Let  $x_0, x_1, x_2, \dots$  be a sequence that converges to  $\xi$  and set  $e_n = \xi - x_n$ . If there exists a number  $P$  and a constant  $C \neq 0$  such that

$$\lim_{n \rightarrow \infty} \frac{|e_{n+1}|}{|e_n|^P} = C,$$

then  $P$  is called the **order of convergence** and  $C$  is called **asymptotic error constant**.

**Examples.**

1. **Fixed point iteration**

$\xi$  fixed point of  $g : I \rightarrow I$  and  $g'(\xi) \neq 0$ .  
 $P = 1$  and  $C = |g'(\xi)|$ .

2. **Newton's method**

$$\lim_{n \rightarrow \infty} \frac{|e_{n+1}|}{|e_n|} = \frac{1}{2} \left| \frac{f''(\xi)}{f'(\xi)} \right|.$$

(If  $\xi$  is a double root, then  $P = 1$ .)

3. **Secant method**

$$|e_{n+1}| = C|e_n||e_{n-1}|$$

$$P = \frac{1+\sqrt{5}}{2} = 1.618\dots$$

$$\lim_{n \rightarrow \infty} \frac{|e_{n+1}|}{|e_n|^P} = \left| \frac{1}{2} \frac{f''(\xi)}{f'(\xi)} \right|^{1/P}, \text{ provided } f'(\xi) \neq 0.$$

**Theorem 1.** Let  $f : [a, b] \rightarrow \mathbb{R}$  be in  $C^2[a, b]$  and let the following conditions be satisfied:

1.  $f(a)f(b) < 0$ ,
2.  $f'(x) \neq 0$ , for all  $x \in [a, b]$ ,
3.  $f''(x)$  doesn't change sign in  $[a, b]$  (might be zero at some points),
- 4.

$$\frac{|f(a)|}{|f'(a)|} \leq b - a \text{ and } \frac{|f(b)|}{|f'(b)|} \leq b - a.$$

Then, the Newton's method converges to the unique solution  $\xi$  of  $f(x) = 0$  in  $[a, b]$  for any choice  $x_0 \in [a, b]$ .

## 6 Solving systems of linear equations

### 6.1 LU Factorisation

We want solve  $Ax = b$  where  $A$  is some known  $n \times n$  matrix,  $b$  a known  $n \times 1$  matrix and  $x$  is unknown.

*Assumption:*  $Ax = b$  can be solved without any row interchange.

We define (finite) sequences of matrices  $A^{(n)} = [a_{ij}^{(n)}]$  and  $b^{(n)}$ .

Define  $A^{(1)} := A$ . Let  $m_{ji} := \frac{a_{ji}^{(1)}}{a_{ii}^{(1)}}$ .

Define  $M^{(1)}$  as

$$M^{(1)} := \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -m_{21} & 1 & 0 & \cdots & 0 \\ -m_{31} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -m_{n-1,1} & 0 & 0 & \cdots & 0 \\ -m_{n1} & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Thus, we can write  $M^{(1)}A^{(1)}x = M^{(1)}b$ .

Let  $A^{(2)} := M^{(1)}A^{(1)}$  and  $b^{(2)} = M^{(1)}b^{(1)}$ .

Note that  $A^{(2)}$  will be a matrix identical to the first one with respect to the last  $n - 1$  columns. However, it's



first column will just have the top element non-zero and everything below will be zero.

We can similarly construct the later matrices that perform the row operations. In general, we have:

$$M^{(k)} := \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & 0 \\ 0 & 0 & \cdots & -m_{k+1,k} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -m_{n,k} & \cdots & 1 \end{bmatrix},$$

along with

$$A^{(k+1)} = M^{(k)} A^{(k)} = M^{(k)} \cdots M^{(1)} A, \text{ and} \\ b^{(k+1)} = M^{(k)} b^{(k)} = M^{(k)} \cdots M^{(1)} b.$$

Finally, set  $U = A^{(n)}$  and  $L = [M^{(1)}]^{-1} \cdots [M^{(n-1)}]^{-1}$ .

Then, we have

$$L = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ m_{21} & 1 & 0 & \cdots & 0 \\ m_{31} & m_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ m_{n-1,1} & m_{n-1,2} & m_{n-1,3} & \cdots & 0 \\ m_{n1} & m_{n2} & m_{n3} & \cdots & 1 \end{bmatrix}.$$

Thus, we have  $A = LU$ . Now, set  $y = Ux$ . We solve  $Ly = b$  for  $y$ . This is easy because  $L$  is lower triangular. Then, we solve  $Ux = y$  for  $x$ .

Check slide 27 of Lecture 11 for example.

LU factorisation requires  $\theta(n^3/3)$  multiplication and division and  $\theta(n^3/3)$  addition and subtraction. However, once the factorisation is done, it can be used again and again to solve  $Ax = b$  for different values of  $b$ . The number of equations then taken to solve  $Ax = b$  is  $\theta(2n^2)$ .

## 6.2 LPU Factorisation

In the previous case, we assumed that we aren't doing any row operations on  $A$  when doing the Gauss elimination. Now, we relax that condition.

Suppose, if possible, we have done some row exchanges while doing Gauss elimination on  $A$ . Construct the matrix  $P$  which is obtained upon doing those exact row exchanges on  $I$ . (Only the row exchanges.)

Suppose that the final product of doing the Gauss elimination following the previous procedure gave us the upper triangular matrix as  $U$  and lower one as  $L$ .

Then, that means  $PA = LU$ . Thus, solving  $Ax = b$  can first be reduced to  $PAx = Pb = b'$ . Now, converting  $PA$  to  $LU$  does not take any row exchange, so we're back in business. (Back to the previous case, that is.)

Check slide 15 of Lecture 12 for example.

## 6.3 Cholesky's Algorithm

**Definition 2.** A matrix  $A$  is positive definite if:

1.  $A = A^t$ , and
2.  $x^t Ax > 0$  for all  $x \neq 0$ .

Given any positive definite matrix  $A$ , we can write  $A = LL^t$ , where  $L$  is lower triangular. (And thus,  $L^t$  would be upper triangular.)

The algorithm to do so is as follows:

Let  $L = (l_{ij})$ . We now construct these entries.

```
set  $l_{ii} := \sqrt{a_{ii}}$ .
for  $j = 2, 3, \dots, n$ :
    set  $l_{j1} := \frac{a_{j1}}{l_{11}}$ .
```

for  $i = 2, 3, \dots, n-1$ :

$$\text{set } l_{ii} := \sqrt{a_{ii} - \sum_{k=1}^{i-1} l_{ik}^2}$$

for  $j = i+1, \dots, n$ :

$$\text{set } l_{ji} := a_{ji} - \frac{\sum_{k=1}^{i-1} l_{jk} l_{ik}}{l_{ii}}.$$

$$\text{set } l_{nn} := \sqrt{a_{nn} - \sum_{k=1}^{n-1} l_{nk}^2}.$$

Note that in the above, we've only defined  $l_{ij}$  for when  $i \geq j$ . The others are obviously 0.

Cholevsky's algorithm requires  $\theta(n^3/6)$  multiplication and division and  $\theta(n^3/6)$  addition and subtraction.

## 6.4 Scaled partial pivoting

Suppose we want to solve  $Ax = b$ . This could lead to round off errors (check slide 17 of Lecture 12). One possible way to combat this is to do the following:

First, define the scale factor  $s_i$  of row  $i$  as the maximum modulus of any element in the row. More precisely,  $s_i := \max_{1 \leq j \leq n} |a_{ij}|$ .

(Note that we assume that  $A$  is invertible and thus, every  $s_i$  will be nonzero.)

Now, along the first column, we find the row which has the greatest ratio  $\frac{|a_{k1}|}{s_k}$ . Suppose this is achieved for row  $p$ , that is,

$$\frac{|a_{p1}|}{s_p} = \max_{1 \leq k \leq n} \frac{|a_{k1}|}{s_k}.$$

If  $p \neq 1$ , then we perform  $R_1 \leftrightarrow R_p$ .

(Now, when we refer to  $s_p$ , we will mean the scale factor of the new  $p$ , that is, the original  $s_1$ . Similarly, for  $s_1$ .) Now, we make everything below  $a_{11}$  zero using the standard row operation.

Now, we repeat the same thing by going along column 2 and finding the row which has the greatest ratio  $\frac{|a_{k2}|}{s_k}$ . If the row is not 2, then we perform the interchange and go on.

Two things I would like to point out:

1. We never change the value of  $s_i$  except the interchanging that we do. In particular, after doing the row operations like  $R_2 - m_{21}R_1$ , I will **not** recalculate the value of  $s_2$ .
2. When considering the ratios  $\frac{|a_{ki}|}{s_k}$  for column  $i$ , we will consider the  $a_{ki}$  that is currently present. That is, in this case, we will consider the values that we get after performing all the operations that have been performed until that point.

Consider the example given in slide 22 of Lecture 12. After doing  $R_1 \leftrightarrow R_3$ ,  $R_2 - \frac{4.01}{1.09}R_1$ , and  $R_3 - \frac{2.11}{1.09}R_1$ , we *do not* recalculate  $s_i$ . (We do exchange the values.)

However, when considering the ratios, we consider the new matrix for taking  $a_{k2}$  obtained after the above subtractions.