UMC202: Review Notes

Naman Mishra

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1 Root-finding Methods

Definition 1.1 (Rate of convergence)**.** Let $\{\alpha\}_{n=1}^{\infty}$ and $\{\beta\}_{n=1}^{\infty}$ be sequences that converge to α and 0 respectively. If $k \in \mathbb{R}^+$ and $n \in \mathbb{N}^+$ exists such that

$$|\alpha_{n+1} - \alpha| \leq k|\beta_n| \quad \text{for all } n \geq N,$$

then $\{\alpha_{n+1}\}$ is said to converge to α with rate of convergence $O(\beta_n)$ and written as

$$\alpha_n = \alpha + O(\beta_n).$$

Definition 1.2 (Order of convergence)**.** Let $\{p_n\}_{n=0}^{\infty}$ converge to p but never equal it. If positive constants α and λ exist with

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^{\alpha}} = \lambda,$$

then $\{p_n\}$ is said to converge to p *of order* α with *asymptotic error constant* λ.

Remarks. If $\alpha = 1$, $\{p_n\}$ is said to converge *linearly* to p.
If $\alpha = 2$, $\{p_n\}$ is said to converge *quadratically* to p.

1.1 Bisection Method

An algorithm is described in algorithm 1.

Theorem 1.3 (Convergence)**.** Suppose that $f \in C^0[a,b]$ and $f(a)f(b) < 0$. Then the bisection method generates a sequence $\{p_n\}_{n=1}^{\infty}$ that converges to a root p of f with

$$|p_n - p| \leq \frac{b-a}{2^n} \quad \text{for all } n.$$

Proof. Induction. □

1.2 Fixed Point Iteration

Definition 1.4 (Fixed point)**.** A number p is said to be a fixed point of a function g if $g(p) = p$.

Theorem 1.5. Let $g : [a,b] \to [a,b]$ be continuous. Then g has a fixed point in $[a,b]$.

Moreover, if g is differentiable on (a,b) with $g'(x) < 1$ for all $x \in (a,b)$, then the fixed point is unique.

Proof. Let $g : [a,b] \to [a,b]$ be continuous. If $g(a) = a$ or $g(b) = b$, we are done. Otherwise, $g(a) - a > 0$ and $g(b) - b < 0$. By IVT, there exists $p \in (a,b)$ such that $g(p) = p$.

Now suppose that g' exists on (a,b) with $g' < 1$. Let $x, y \in (a,b)$ be fixed points of g. If they are distinct, then by MVT, there exists $c \in (x,y)$ such that

$$g'(c) = \frac{g(y) - g(x)}{y - x} = \frac{y - x}{y - x} = 1,$$

which is a contradiction. □

The fixed point iteration method is described in algorithm 2.

Theorem 1.6 (Fixed point theorem)**.** Let $g \in C^0[a,b]$ be such that $g(x) \in [a,b]$ for all $x \in [a,b]$. Suppose further that g is differentiable on (a,b) and that a constant $0 < k < 1$ exists with $g'(x) \le k < 1$ for all $x \in (a,b)$.

Then for any $p_0 \in [a,b]$, the sequence $\{p_n\}_{n=1}^{\infty}$ generated by $p_n = g(p_{n-1})$ converges to the unique fixed point p in $[a,b]$ with rate of convergence $O(k^n)$.

Proof. Let p be the unique fixed point of g in $[a,b]$, whose existence is guaranteed by theorem 1.5.

Let $p_0 \in [a,b]$. Then for any $n \in \mathbb{N}^+$, there exists by MVT a $c_n \in (a,b)$ such that

$$\frac{|g(p_n) - g(p)|}{|p_n - p|} = \frac{|p_{n+1} - p|}{|p_n - p|} = |g'(c_n)| \le k.$$

Thus by induction,

$$|p_n - p| \le k^n |p_0 - p| \le k^n \max\{p_0 - a, b - p_0\}. \qquad \square$$

Corollary 1.7. If g satisfies the hypotheses of theorem 1.6, then for any $p_0 \in [a,b]$,

$$\begin{aligned} |p_n - p| &\le k^n \max\{p_0 - a, b - p_0\}, \text{ and} \\ |p_n - p| &\le \frac{k^n}{1-k} |p_1 - p_0|. \end{aligned}$$

Proof. The first inequality is proved in the proof of theorem 1.6.

For the second inequality, note that

$$\begin{aligned} |p_0 - p| &= |p_0 - p_1 + p_1 - p| \\ &\le |p_0 - p_1| + |p_1 - p| \\ &\le |p_0 - p_1| + k|p_0 - p| \\ \implies |p_0 - p| &\le \frac{1}{1-k}|p_1 - p_0|. \end{aligned}$$

Thus using

$$|p_n - p| \le k^n |p_0 - p|$$

we get

$$|p_n - p| \leq \frac{k^n}{1-k}|p_1 - p_0|. \qquad \square$$

1.3 Newton-Raphson Method

Fixed point iteration with $g(x) = x - \frac{f(x)}{f'(x)}$. An algorithm is described in algorithm 3.

Theorem 1.8 (Convergence)**.** Let $f \in C^2[a,b]$ have a root p in $[a,b]$ such that $f'(p) \neq 0$. Then there exists a $\delta > 0$ such that for any $p_0 \in N_\delta(p)$, the sequence $\{p_n\}_{n=1}^\infty$ generated by Newton's method converges to p.

Proof. Let $g(x) = x - \frac{f(x)}{f'(x)}$. Newton's method is described by $p_n = g(p_{n-1})$ for $n \geq 1$.

Since f' is continuous on $[a,b]$, there exists a $\delta_1 > 0$ such $f'(x) \neq 0$ for all $x \in N_{\delta_1}(p)$. Thus g is defined on $N_{\delta_1}(p)$.

$g'(x) = \frac{f(x)f''(x)}{f'(x)^2}$. Since $f \in C^2[a,b]$, g' is continuous on $N_{\delta_1}(p)$.

Let $0 < k < 1$. Since $g'(p) = 0$ and g' is continuous, there exists a neighborhood $N_\delta(p)$ on which $|g'|$ is bounded by k. By MVT, this implies that g maps $N_\delta(p)$ into itself.

Thus by theorem 1.6, the sequence $\{p_n\}$ converges to the unique fixed point p of g for all initial approximations $p_0 \in N_\delta(p)$. $\square$

Theorem 1.9. Let g follow all hypotheses of theorem 1.6.

If $g'(p) \neq 0$, then for any $p_0 \in N_\delta(p) \backslash \{p\}$, the sequence $p_n = g(p_{n-1})$ converges only linearly to p.

Proof. By MVT,

$$\begin{aligned}
\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|} &= \lim_{n\to\infty} |g'(\xi_n)| \\
&= \left| g'(\lim_{n\to\infty} \xi_n) \right| \\
&= |g'(p)|
\end{aligned}$$

where ξ_n is between p_n and p. $\square$

Theorem 1.10. Let $g \in C^2(I)$ for some open interval I containing a fixed point p of g. Suppose that $g'(p) = 0$.

Then there exists a $\delta > 0$ such that for any $p_0 \in N_\delta(p)$, the sequence $p_n = g(p_{n-1})$ converges at least quadratically to p.

Moreover, if g'' is strictly bounded by M on I, then

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2$$

for large n. (Or even for any n?)

Proof. Let $0 < k < 1$. Choose δ_0 such that $|g'| \leq k$ on $N_{\delta_0}(p)$. Let p_0 be in $N_{\delta_0}(p)$. Then we know from theorem 1.6 that g maps $N_{\delta_0}(p)$ into itself and the sequence $p_n = g(p_{n-1})$ converges to p.

By Taylor's theorem,

$$\begin{aligned} g(p_n) - g(p) &= g'(p)(p_n - p) + \frac{g''(\xi_n)}{2}(p_n - p)^2 \\ p_{n+1} - p &= \frac{g''(\xi_n)}{2}(p_n - p)^2. \end{aligned} \tag{$*$}$$

where ξ_n is between p_n and p. Thus $\lim_{n\to\infty} \xi_n = p$ and since g'' is continuous,

$$\lim_{n\to\infty} \frac{p_{n+1} - p}{(p_n - p)^2} = \frac{g''(p)}{2}$$

and so p_n converges at least quadratically.

If g'' is strictly bounded by M on I, then eq. ($*$) implies that

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2.$$ $\square$

Corollary 1.11. Newton's method exhibits quadratic convergence.

1.4 Secant Method

The secant method is described in algorithm 4.

1.5 Regula Falsi Method

In the bisection method, the root is always bracketed in the interval $[a_n, b_n]$. In the Newton-Raphson and secant methods, no such guarantee is afforded. Regula falsi is a modification of the secant method that guarantees root bracketing. It is described in algorithm 5.

2 Interpolation

Definition 2.1 (Lagrange basis)**.** Let $S = \{x_0, \ldots, x_n\}$ be a set of $n+1$ distinct points in $\mathbb{R}$. Then the *Lagrange basis* $\left\{L_0^S, \ldots, L_n^S\right\}$ is defined as

$$L_i^S(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

for $i \in \{0, \ldots, n\}$.

Theorem 2.2 (Unique interpolation)**.** Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ be a function. Let $S = \{x_0, \ldots, x_n\}$ be distinct points in D. Then there exists a unique polynomial p of degree at most n such that $p(x_i) = f(x_i)$ for all $i \in \{0, \ldots, n\}$, given by

$$p(x) = \sum_{i=0}^{n} f(x_i) L_i^S(x).$$

Proof. **Existence:** Note that $L_i^S(x_i) = \prod_{j\neq i} \frac{x_i - x_j}{x_i - x_j} = 1$ and for $i \neq k$,

$$\begin{aligned}
L_i^S(x_k) &= \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x_k - x_j}{x_i - x_j} \\
&= \prod_{\substack{j=0 \\ j\neq i,k}}^{n} \frac{x_k - x_j}{x_i - x_j} \cdot \frac{x_k - x_k}{x_i - x_k} \\
&= 0.
\end{aligned}$$

Thus

$$\begin{aligned}
p(x_k) &= \sum_{i=0}^{n} f(x_i) L_i^S(x_k) \\
&= \sum_{i=0}^{n} f(x_i) \delta_{ik} \\
&= f(x_k)
\end{aligned}$$

where δ is the Kronecker delta.

Uniqueness: Suppose that p and q are polynomials of degree at most n that agree with f at $x_0, \ldots, x_n$. Then $r = p - q$ is a polynomial of degree at most n that has at least $n+1$ roots. By the fundamental theorem of algebra, r is the zero polynomial. $\square$

Corollary 2.3. Lagrange basis polynomials form a basis for $\mathcal{P}_n$, the space of polynomials of degree at most n.

Proof. Let $S = \{x_0, \ldots, x_n\}$ be distinct points in $\mathbb{R}$. Let p be a polynomial of degree at most n. Then $p = \sum_{i=0}^{n} p(i) L_i^S$.

Thus the Lagrange basis polynomials span the space. Since $\dim \mathcal{P}_n = n+1$, they form a basis. $\square$

Definition 2.4 (Newton basis)**.** Let $S = \{x_0, \ldots, x_n\}$ be a set of $n+1$ distinct points in $\mathbb{R}$. Then the *Newton basis* $\left\{N_0^S, \ldots, N_n^S\right\}$ is defined as

$$N_i^S(x) = \prod_{j=0}^{i-1} (x - x_j)$$

for $i \in \{0, \ldots, n\}$.

Theorem 2.5. The Newton basis $\left\{N_0^S, \ldots, N_n^S\right\}$ is a basis for $\mathcal{P}_n$.

3 Initial Value Problem

3.1 Central differences

From Taylor's theorem,

$$\begin{aligned}
y_{i+1} &= y_i + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \frac{h^3}{3!}y'''(\xi_i) \\
y_{i-1} &= y_i - hy'(t_i) + \frac{h^2}{2}y''(t_i) - \frac{h^3}{3!}y'''(\eta_i) \\
y_{i+1} - y_{i-1} &= 2hy'(t_i) + \frac{h^3}{3!}(y'''(\xi_i) + y'''(\eta_i))
\end{aligned}$$

Dropping the remainder term gives the central differences scheme.

$$\begin{aligned}
w_0 &= \alpha \\
w_1 &= \alpha_1 \\
w_{i+1} &= w_{i-1} + 2hf(t_i, w_i)
\end{aligned}$$

3.2 Stability

3.2.1 Multistep methods

Definition 3.1 (Characteristic polynomial)**.** For the multistep method $w_0 = \alpha, w_1 = \alpha_1, \ldots, w_n = \alpha_n$ and

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m}),$$

we define the characteristic polynomial P as

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_0.$$

The stability of the multistep method with respect to round off errors is dictated by the magnitudes of the roots of P.

Definition 3.2 (Root condition)**.** Let $\lambda_1, \ldots, \lambda_n$ be the n roots of the characteristic polynomial equation

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_0 = 0.$$

associated with the multistep method described above.

If $|\lambda_i| \leq 1$ and all roots with magnitude 1 are simple, then the difference method is said to satisfy the *root condition*.

Definition 3.3.

- A multistep method that satisfies the root condition and has 1 as the only root of magnitude 1 is said to be *strongly stable*.
- A multistep method that satisfies the root condition and has more than one distinct root of magnitude 1 is said to be *weakly stable*.
- A multistep method that does not satisfy the root condition is said to be *unstable*.

4 Algorithms

Algorithm 1 Bisection method of finding a root

Require: A continuous function f on $[a, b]$ such that $f(a)f(b) < 0$, a tolerance $\varepsilon > 0$, and a maximum number of iterations N

Ensure: An approximate root of f on $[a, b]$, or Nil if not found

for $i \leftarrow 1$ to N **do**
    $p \leftarrow \frac{a+b}{2}$
    $f_p \leftarrow f(p)$
    if $f_p = 0$ or $\frac{b-a}{2} < \varepsilon$ **then**
        return p
    if $f(a) \cdot f_p < 0$ **then**
        $b \leftarrow p$
    else
        $a \leftarrow p$
return Nil

Algorithm 2 Fixed point iteration method of finding a root

Require: A function $g : [a, b] \to [a, b]$ that follows the conditions of theorem 1.6, an initial guess $p_0 \in [a, b]$, a tolerance $\varepsilon > 0$, and a maximum number of iterations N

Ensure: An approximate fixed point of g on $[a, b]$, or NIL if not found

for $i \leftarrow 1$ to N **do**
    $p \leftarrow g(p_0)$
    if $|p - p_0| < \varepsilon$ **then**
        return p
    $p_0 \leftarrow p$
return NIL

Algorithm 3 Newton-Raphson method for finding a root

Require: A function f that follows the hypotheses of theorem 1.8, an initial guess p_0, a tolerance $\varepsilon > 0$, and a maximum number of iterations N

Ensure: An approximate root of f, or NIL if not found

for $i \leftarrow 1$ to N **do**
    $p \leftarrow p_0 - \frac{f(p_0)}{f'(p_0)}$
    if $|p - p_0| < \varepsilon$ **then**
        return p
    $p_0 \leftarrow p$
return NIL

Algorithm 4 Secant method for finding a root

Require: A function f that follows God knows what conditions, initial guesses p_0 and p_1, a tolerance $\varepsilon > 0$, and a maximum number of iterations N

Ensure: An approximate root of f, or NIL if not found

$(q_0, q_1) \leftarrow (f(p_0), f(p_1))$
for $i \leftarrow 2$ to N **do**
    $p \leftarrow \frac{p_0 q_1 - p_1 q_0}{q_1 - q_0}$ $\triangleright$ *External $q_0 : q_1$? Or internal $|q_0| : |q_1|$?*
    $(p_0, q_0) \leftarrow (p_1, q_1)$
    $(p_1, q_1) \leftarrow (p, f(p))$
    if $q_1 = 0$ or $|p_1 - p_0| < \varepsilon$ **then**
        return p_1
return NIL

Algorithm 5 Regula falsi method for finding a root

Require: A function f that follows God knows what conditions, initial guesses p_0 and p_1, a tolerance $\varepsilon > 0$, and a maximum number of iterations N

Ensure: An approximate root of f, or NIL if not found

$(q_0, q_1) \leftarrow (f(p_0), f(p_1))$
for $i \leftarrow 2$ to N **do**
    $p \leftarrow \frac{p_0 q_1 - p_1 q_0}{q_1 - q_0}$
    $q \leftarrow f(p)$
    if $q = 0$ or $|p - p_1| < \varepsilon$ **then**
        return p
    if $q_0 \cdot q < 0$ **then**
        $(p_1, q_1) \leftarrow (p, q)$
    else
        $(p_0, q_0) \leftarrow (p, q)$
return NIL