Solving Non-linear Equations (20 points)

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Question: Why we need iterative methods?

> If f is a general nonlinear function, there is no formula exists for finding roots of $f(x) = 0$, **iterative methods** will be used to compute **approximate roots**

Three algorithms:

Bisection algorithm:

Algorithm 1 Bisection algorithm

Input: $f(x)$ $[a, b]$ with $f(a) \cdot f(b) < 0$ the tolerance δ
$c \leftarrow \frac{a+b}{2}$ ▷ c is the root we will return
$\textit{error bound} \leftarrow \frac{|b-a|}{2}$
while $\textit{error bound} > \delta$ **do**
  if $f(c) = 0$ **then**
    we say c is the root, stop.
  else
    if $f(a) \cdot f(c) < 0$ **then**
      $b \leftarrow c$
    else
      $a \leftarrow c$
    end if
  end if
  $c \leftarrow \frac{a+b}{2}$
  $\textit{error bound} \leftarrow \frac{\textit{error bound}}{2}$
end while
return c

Newton's Method:

Algorithm 2 Newton's algorithm

Input: $f(x) \quad f'(x), x, xtol, ftol, n_{max}$ ▷ $x \rightarrow$ initial point
▷ $n_{max} \rightarrow$ maximum number of iterations
for $n = 1 : n_{max}$ **do**

$\quad d \leftarrow \dfrac{f(x)}{f'(x)}$

$\quad x \leftarrow x - d$
$\quad$ **if** $|d| \leq xtol$ *or* $|f(x)| \leq ftol$ **then**
$\quad\quad root \leftarrow x$
$\quad\quad$ stop
$\quad$ **end if**

end for
$root \leftarrow x$

Stop Criteria:

- $|x_{n+1} - x_n| \leq xtol$
- $|f_{n+1}| \leq ftol$
- The maximum number of iteration reached

Newton's Method's Iteration formula:

Given a point x_0, we do Taylor Expansion about x_0:

$$f(x) = f(x_0) + f'(x_0) \cdot (x - x_0) + \frac{f''(z)}{2}(x - x_0)^2$$

where $z \in (x, x_0)$

We use $\ell(x) = f(x_0) + f'(x_0) \cdot (x - x_0)$ as an approximation of $f(x)$. In order to solve $f(x) = 0$, we try to solve $\ell(x) = 0$

$$\ell(x) = 0 \implies f(x_0) + f'(x_0) \cdot (x - x_0) = 0 \implies x = x_0 - \frac{f(x_0)}{f'(x_0)}$$

We choose $x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$ as our approximate root of $f(x) = 0$
If this x_1 is not a good approximate root, we continue this iteration. In general, we have the Newton iteration:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Secant Method:

Sometimes, the derivative of a function is really hard or even impossible to compute, then, we try to use **divided difference** to replace $f'(x_n)$. Then we get our secant iteration:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad \text{use } \textbf{divided difference} \text{ to replace } f'(x_n) \implies \boxed{x_{n+1} = x_n - \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \cdot f(x_n)}$$

Algorithm 3 Secant's algorithm

Input: $f(x), x_0, x_1, xtol, ftol, n_{max}$ ▷ $x_0, x_1 \rightarrow$ initial point
▷ $n_{max} \rightarrow$ maximum number of iterations
for $n = 1 : n_{max}$ **do**
  $d \leftarrow \dfrac{x_1 - x_0}{f(x_1) - f(x_0)} \cdot f(x_1)$
  $x_0 \leftarrow x_1$
  $f(x_0) \leftarrow f(x_1)$
  $x_1 \leftarrow x_1 - d$
  $fx_1 = f(x_1)$
  if $|d| \le xtol$ *or* $|fx_1| \le ftol$ **then**
    $root \leftarrow x_1$
    stop
  end if
end for
$root \leftarrow x_1$

Comparison of the Three Methods:

- The Bisection Method:
  - Advantage: Simple, guaranteed to converge, applicable to non-smooth functions
  - Disadvantage: Linear convergence
- Newton's Method:
  - Advantage: Quadratic convergence
  - Disadvantage: need to compute f' may not converge
- The Secant Method:
  - Advantage: Super-Linear convergence no need to compute f'
  - Disadvantage: slower than NM may not converge

Convergence Analysis:

Quadratic Convergence: A sequence $\{x_n\}$ is said o have quadratic convergence to x if:

$$\lim_{n\to\infty} \frac{|x_{n+1} - x|}{|x_n - x|^2} = c$$

where c is some finite non-zero constant.

Suppose r is a root of $f(x) = 0$ and x_n converges to r.
We do Taylor series expansion about x_n

$$f(r) = f(x_n) + (r - x_n)f'(x_n) + \frac{(r - x_n)^2}{2} f''(z_n)$$

where z_n is between r and x_n.

Divide both sides by $f'(x_n)$ and use the fact r is the root of $f(x) = 0$, then we have:

$$0 = \frac{f(x_n)}{f'(x_n)} + (r - x_n) + (r - x_n)^2 \cdot \frac{f''(z_n)}{2f'(x_n)}$$

As we use Newton's Method, we have $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$, then we have:

$$0 = x_n - x_{n+1} + (r - x_n) + (r - x_n)^2 \cdot \frac{f''(z_n)}{2f'(x_n)} \implies r - x_{n+1} = c_n \cdot (r - x_n)^2, \quad c_n = -\frac{f''(z_n)}{2f'(x_n)}$$

As we said before, $x_n \to r$ and z_n is between x_n and r, thus we have $z_n \to r$ and then, we have:

$$\lim_{n\to\infty} \frac{|r - x_{n+1}|}{|r - x_n|^2} = \lim_{n\to\infty} |c_n| = |\frac{f''(r)}{2f'(r)}| = c$$

Show that $\lim_{n\to\infty} |\dfrac{f(x_{n+1})}{f(x_n)}| = c$

We expand the Taylor Series as following:

$$f(x_{n+1}) = f(x_n) + (x_{n+1} - x_n) \cdot f'(x_n) + \frac{(x_{n+1} - x_n)^2}{2} \cdot f''(z_n) \; where \; z_n \text{ is between } x_n \; and \; x_{n+1}$$

According to Newton Iteration, we have:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \implies x_n - x_{n+1} = \frac{f(x_n)}{f'(x_n)}$$

Thus, we have:

$$f(x_{n+1}) = f(x_n) - f(x_n) + \frac{1}{2} \cdot \frac{f(x_n)^2}{f'(x_n)^2} \cdot f''(z_n)$$

$$\frac{f(x_{n+1})}{f(x_n)^2} = \frac{1}{2} \cdot \frac{f''(z_n)}{f'(x_n)^2}$$

As, we know, z_n is between x_n *and* x_{n+1}, when $n \to \infty$, we have x_n and x_{n+1} converges to root r, which means, $z_n \to r$

Thus, we have:

$$\lim_{n\to\infty} \frac{|f(x_{n+1})|}{|f(x_n)^2|} = \lim_{n\to\infty} \frac{1}{2} \cdot \frac{|f''(z_n)|}{|f'(x_n)|^2} = \frac{1}{2} \cdot \frac{|f''(r)|}{|f'(r)|^2} = c \neq 0$$

Some Questions about this Chapter:

1 Under which cases, NM and SM are not converge?
Answer: the initial point is not close to the root r

2 Do we need to know how to derive the convergence rate of Bisection is linear? (No.)

Usually? What about unusual case?

$$c = |\frac{f''(r)}{2f'(r)}|$$

So, could I say unusual case always comes from one of $f''(r)$ $f'(r) = 0$

$f''(r) = 0 \implies$ converge faster than quadratic
$f'(r) = 0 \implies$ converge at linear convergence rate, but why?

For $f(x) = (x-1)^2$, it converges at linear rate.
What we want to prove is that

$$\lim_{n\to\infty} \frac{|x_{n+1} - x|}{|x_n - x|} = \text{some constant } c \tag{1}$$

As we used in Newton method:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{(x_n - 1)^2}{2 \cdot (x_n - 1)} = x_n - \frac{x_n - 1}{2} = \frac{x_n + 1}{2}$$

Thus, we substitute this into Equation(1):

$$\lim_{n\to\infty} |\frac{\frac{x_n + 1}{2} - 1}{x_n - 1}| = \frac{1}{2}$$

For $f(x) = \sin(x)$, it converges faster than Quadratic Rate.
What we want to prove is that

$$\lim_{n\to\infty} \frac{|x_{n+1} - x|}{|x_n - x|^k} = \text{some constant } c \tag{2}$$

As we used in Newton method:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{\cos(x_n)}{\sin(x_n)}$$

Thus, we substitute this into Equation(2):

$$\lim_{n\to\infty} \frac{|x_{n+1} - x|}{|x_n - x|^k} = \frac{|x_n - \dfrac{\cos(x_n)}{\sin(x_n)} - \pi|}{|x_n - \pi|^k}$$