Chapter 2
Solutions of Equations in One Variable

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The Bisection Method

Suppose $f$ continuous on $[a, b]$, and $f(a), f(b)$ opposite signs

By the IVT, there exists an $x$ in $(a, b)$ with $f(x) = 0$

Divide the interval $[a, b]$ by computing the midpoint

$$p = (a + b)/2$$

If $f(p)$ has same sign as $f(a)$, consider new interval $[p, b]$
If $f(p)$ has same sign as $f(b)$, consider new interval $[a, p]$

Repeat until interval small enough to approximate $x$ well
function p = bisection(f, a, b, tol)
% Solve f(p) = 0 using the bisection method.

while 1
    p = (a+b) / 2;
    if p−a < tol, break; end
    if f(a)*f(p) > 0
        a = p;
    else
        b = p;
    end
end
Termination Criteria

- Many ways to decide when to stop:

\[
\frac{|p_N - p_{N-1}|}{|p_N|} < \varepsilon \\
|f(p_N)| < \varepsilon \\
|p_N - p_{N-1}| < \varepsilon
\]

- None is perfect, use a combination in real software
Suppose that \( f \in C[a, b] \) and \( f(a) \cdot f(b) < 0 \). The Bisection method generates a sequence \( \{p_n\}_{n=1}^{\infty} \) approximating a zero \( p \) of \( f \) with
\[
|p_n - p| \leq \frac{b - a}{2^n}, \quad \text{when } n \geq 1.
\]

The sequence \( \{p_n\}_{n=1}^{\infty} \) converges to \( p \) with rate of convergence \( O(1/2^n) \):
\[
p_n = p + O \left( \frac{1}{2^n} \right).
\]
A number $p$ is a *fixed point* for a given function $g$ if $g(p) = p$.

Given a root-finding problem $f(p) = 0$, there are many $g$ with fixed points at $p$:

- $g(x) = x - f(x)$
- $g(x) = x + 3f(x)$
- ...  

If $g$ has fixed point at $p$, then $f(x) = x - g(x)$ has a zero at $p$. 
Existence and Uniqueness of Fixed Points

**Theorem**

a. If $g \in C[a, b]$ and $g(x) \in [a, b]$ for all $x \in [a, b]$, then $g$ has a fixed point in $[a, b]$.

b. If, in addition, $g'(x)$ exists on $(a, b)$ and a positive constant $k < 1$ exists with

$$|g'(x)| \leq k,$$

for all $x \in (a, b)$,

then the fixed point in $[a, b]$ is unique.
Fixed-Point Iteration

For initial \( p_0 \), generate sequence \( \{p_n\}_{n=0}^{\infty} \) by \( p_n = g(p_{n-1}) \).

If the sequence converges to \( p \), then

\[
p = \lim_{n \to \infty} p_n = \lim_{n \to \infty} g(p_{n-1}) = g \left( \lim_{n \to \infty} p_{n-1} \right) = g(p).
\]

MATLAB Implementation

```matlab
function p = fixedpoint(g, p0, tol)
% Solve g(p) = p using fixed-point iteration.

while 1
    p = g(p0);
    if abs(p-p0) < tol, break; end
    p0 = p;
end
```
Theorem (Fixed-Point Theorem)

Let \( g \in C[a, b] \) be such that \( g(x) \in [a, b] \), for all \( x \) in \( [a, b] \). Suppose, in addition, that \( g' \) exists on \((a, b)\) and that a constant \( 0 < k < 1 \) exists with

\[
|g'(x)| \leq k, \quad \text{for all } x \in (a, b).
\]

Then, for any number \( p_0 \) in \([a, b]\), the sequence defined by \( p_n = g(p_{n-1}) \) converges to the unique fixed point \( p \) in \([a, b]\).

Corollary

If \( g \) satisfies the hypotheses above, then bounds for the error are given by

\[
|p_n - p| \leq k^n \max\{p_0 - a, b - p_0\}
\]

\[
|p_n - p| \leq \frac{k^n}{1 - k} |p_1 - p_0|
\]
Newton's Method

**Taylor Polynomial Derivation**

Suppose $f \in C^2[a, b]$ and $p_0 \in [a, b]$ approximates solution $p$ of $f(x) = 0$ with $f'(p_0) \neq 0$. Expand $f(x)$ about $p_0$:

$$f(p) = f(p_0) + (p - p_0)f'(p_0) + \frac{(p - p_0)^2}{2}f''(\xi(p))$$

Set $f(p) = 0$, assume $(p - p_0)^2$ negligible:

$$p \approx p_1 = p_0 - \frac{f(p_0)}{f'(p_0)}$$

This gives the sequence $\{p_n\}_{n=0}^{\infty}$:

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$
Newton’s Method

MATLAB Implementation

function p = newton(f, df, p0, tol)
% Solve f(p) = 0 using Newton's method.

while 1
    p = p0 - f(p0)/df(p0);
    if abs(p - p0) < tol, break; end
    p0 = p;
end
Newton’s Method – Convergence

Fixed Point Formulation

Newton’s method is fixed point iteration $p_n = g(p_{n-1})$ with

$$g(x) = x - \frac{f(x)}{f'(x)}$$

Theorem

Let $f \in C^2[a, b]$. If $p \in [a, b]$ is such that $f(p) = 0$ and $f'(p) \neq 0$, then there exists a $\delta > 0$ such that Newton’s method generates a sequence $\{p_n\}_{n=1}^{\infty}$ converging to $p$ for any initial approximation $p_0 \in [p - \delta, p + \delta]$. 
Variations without Derivatives

The Secant Method

Replace the derivative in Newton’s method by

\[ f'(p_{n-1}) \approx \frac{f(p_{n-2}) - f(p_{n-1})}{p_{n-2} - p_{n-1}} \]

to get

\[ p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})} \]

The Method of False Position (Regula Falsi)

Like the Secant method, but with a test to ensure the root is bracketed between iterations.
Definition

Suppose \( \{p_n\}_{n=0}^{\infty} \) is a sequence that converges to \( p \), with \( p_n \neq p \) for all \( n \). If positive constants \( \lambda \) and \( \alpha \) exist with

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

then \( \{p_n\}_{n=0}^{\infty} \) converges to \( p \) of order \( \alpha \), with asymptotic error constant \( \lambda \).

An iterative technique \( p_n = g(p_{n-1}) \) is said to be of order \( \alpha \) if the sequence \( \{p_n\}_{n=0}^{\infty} \) converges to the solution \( p = g(p) \) of order \( \alpha \).

Special cases

- If \( \alpha = 1 \) (and \( \lambda < 1 \)), the sequence is linearly convergent
- If \( \alpha = 2 \), the sequence is quadratically convergent
Fixed Point Convergence

Theorem

Let \( g \in C[a, b] \) be such that \( g(x) \in [a, b] \), for all \( x \in [a, b] \).
Suppose \( g' \) is continuous on \((a, b)\) and that \( 0 < k < 1 \) exists with
\[ |g'(x)| \leq k \]
for all \( x \in (a, b) \). If \( g'(p) \neq 0 \), then for any number \( p_0 \)
in \( [a, b] \), the sequence \( p_n = g(p_{n-1}) \) converges only linearly to the
unique fixed point \( p \) in \([a, b] \).

Theorem

Let \( p \) be solution of \( x = g(x) \). Suppose \( g'(p) = 0 \) and \( g'' \)
continuous with \( |g''(x)| < M \) on open interval \( I \) containing \( p \).
Then there exists \( \delta > 0 \) s.t. for \( p_0 \in [p - \delta, p + \delta] \), the sequence
defined by \( p_n = g(p_{n-1}) \) converges at least quadratically to \( p \), and
\[ |p_{n+1} - p| < \frac{M}{2} |p_n - p|^2. \]
Newton’s Method as Fixed-Point Problem

Derivation

Seek \( g \) of the form

\[
  g(x) = x - \phi(x)f(x).
\]

Find differentiable \( \phi \) giving \( g'(p) = 0 \) when \( f(p) = 0 \):

\[
  g'(x) = 1 - \phi'(x)f(x) - f'(x)\phi(x)
\]
\[
  g'(p) = 1 - \phi'(p) \cdot 0 - f'(p)\phi(p)
\]

and \( g'(p) = 0 \) if and only if \( \phi(p) = 1/f'(p) \). This gives Newton’s method

\[
  p_n = g(p_{n-1}) = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}
\]
Definition
A solution $p$ of $f(x) = 0$ is a zero of multiplicity $m$ of $f$ if for $x \neq p$, we can write $f(x) = (x - p)^m q(x)$, where $\lim_{x \to p} q(x) \neq 0$.

Theorem
$f \in C^1[a, b]$ has a simple zero at $p$ in $(a, b)$ if and only if $f(p) = 0$, but $f'(p) \neq 0$.

Theorem
The function $f \in C^m[a, b]$ has a zero of multiplicity $m$ at point $p$ in $(a, b)$ if and only if

$$0 = f(p) = f'(p) = f''(p) = \cdots = f^{(m-1)}(p), \text{ but } f^{(m)}(p) \neq 0.$$
Newton’s Method for Multiple Roots

Define $\mu(x) = \frac{f(x)}{f'(x)}$. If $p$ is a zero of $f$ of multiplicity $m$ and $f(x) = (x - p)^m q(x)$, then

$$\mu(x) = (x - p) \frac{q(x)}{mq(x) + (x - p)q'(x)}$$

also has a zero at $p$. But $q(p) \neq 0$, so

$$\frac{q(p)}{mq(p) + (p - p)q'(p)} = \frac{1}{m} \neq 0,$$

and $p$ is a simple zero of $\mu$. Newton’s method can then be applied to $\mu$ to give

$$g(x) = x - \frac{f(x)f'(x)}{[f'(x)]^2 - f(x)f''(x)}$$
Aitken’s $\Delta^2$ Method

Accelerating linearly convergent sequences

- Suppose $\{p_n\}_{n=0}^\infty$ linearly convergent with limit $p$
- Assume that

$$\frac{p_{n+1} - p}{p_n - p} \approx \frac{p_{n+2} - p}{p_{n+1} - p}$$

- Solving for $p$ gives

$$p \approx \frac{p_{n+2}p_n - p_{n+1}^2}{p_{n+2} - 2p_{n+1} + p_n} = \cdots = p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}$$

- Use this for new more rapidly converging sequence $\{\hat{p}_n\}_{n=0}^\infty$:

$$\hat{p}_n = p_n - \frac{(p_{n+1} - p)^2}{p_{n+2} - 2p_{n+1} + p_n}$$
Delta Notation

Definition

For a given sequence \( \{p_n\}_{n=0}^\infty \), the forward difference \( \Delta p_n \) is defined by

\[
\Delta p_n = p_{n+1} - p_n, \quad \text{for } n \geq 0
\]

Higher powers of the operator \( \Delta \) are defined recursively by

\[
\Delta^k p_n = \Delta (\Delta^{k-1} p_n), \quad \text{for } k \geq 2
\]

Aitken's \( \Delta^2 \) method using delta notation

Since \( \Delta^2 p_n = p_{n+2} - 2p_{n+1} + p_n \), we can write

\[
\hat{p}_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n}, \quad \text{for } n \geq 0
\]
Convergence of Aitken’s $\Delta^2$ Method

**Theorem**

Suppose that $\{p_n\}_{n=0}^{\infty}$ converges linearly to $p$ and that

$$\lim_{n \to \infty} \frac{p_{n+1} - p}{p_n - p} < 1$$

Then $\{\hat{p}_n\}_{n=0}^{\infty}$ converges to $p$ faster than $\{p_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n \to \infty} \frac{\hat{p}_n - p}{p_n - p} = 0$$
Steffensen’s Method

Accelerating fixed-point iteration

Aitken’s $\Delta^2$ method for fixed-point iteration gives

$$p_0, \ p_1 = g(p_0), \ p_2 = g(p_1), \ \hat{p}_0 = \{\Delta^2\}(p_0),$$
$$p_3 = g(p_2), \ \hat{p}_1 = \{\Delta^2\}(p_1), \ \ldots$$

Steffensen’s method assumes $\hat{p}_0$ is better than $p_2$:

$$p^{(0)}_0, \ p^{(0)}_1 = g(p^{(0)}_0), \ p^{(0)}_2 = g(p^{(0)}_1), \ p^{(1)}_0 = \{\Delta^2\}(p^{(0)}_0),$$
$$p^{(1)}_1 = g(p^{(1)}_0), \ \ldots$$

Theorem

Suppose $x = g(x)$ has solution $p$ with $g'(p) \neq 1$. If exists $\delta > 0$ s.t. $g \in C^3[p - \delta, p + \delta]$, then Steffensen’s method gives quadratic convergence for $p_0 \in [p - \delta, p + \delta]$. 
function p = steffensen(g, p0, tol)
% Solve g(p) = p using Steffensen's method.

while 1
    p1 = g(p0);
    p2 = g(p1);
    p = p0 - (p1 - p0)^2 / (p2 - 2*p1 + p0);
    if abs(p - p0) < tol, break; end
    p0 = p;
end
Zeros of Polynomials

**Polynomial**

A polynomial of degree \( n \) has the form \( P(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 \) with coefficients \( a_i \) and \( a_n \neq 0 \).

**Theorem (Fundamental Theorem of Algebra)**

If \( P(x) \) polynomial of degree \( n \geq 1 \), with real or complex coefficients, \( P(x) = 0 \) has at least one root.

**Corollary**

Exists unique \( x_1, \ldots, x_k \) and \( m_1, \ldots, m_k \), with \( \sum_{i=1}^{k} m_i = n \) and

\[
P(x) = a_n (x - x_1)^{m_1} (x - x_2)^{m_2} \cdots (x - x_k)^{m_k}.
\]

**Corollary**

\( P(x), Q(x) \) polynomials of degree at most \( n \). If \( P(x_i) = Q(x_i) \) for \( i = 1, 2, \ldots, k \), with \( k > n \), then \( P(x) = Q(x) \).
Horner’s Method

**Theorem (Horner’s Method)**

Let \( P(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 \). If \( b_n = a_n \) and

\[
 b_k = a_k + b_{k+1} x_0, \quad \text{for} \ k = n - 1, n - 2, \ldots, 1, 0,
\]

then \( b_0 = P(x_0) \). Moreover, if

\[
 Q(x) = b_n x^{n-1} + b_{n-1} x^{n-2} + \cdots + b_2 x + b_1,
\]

then \( P(x) = (x - x_0) Q(x) + b_0 \).

**Computing Derivatives**

Differentiation gives

\[
 P'(x) = Q(x) + (x - x_0) Q'(x) \quad \text{and} \quad P'(x_0) = Q(x_0).
\]
function [y, z] = horner(a, x)
% Evaluate polynomial y(x) using Horner's method.

n = length(a)−1;
y = a(1);
z = a(1);
for j = 2:n
    y = x*y + a(j);
    z = x*z + y;
end
y = x*y + a(n+1);
Compute approximate root $\hat{x}_1$ using Newton. Then

\[ P(x) \approx (x - \hat{x}_1)Q_1(x). \]

Apply recursively on $Q_1(x)$ until the quadratic factor $Q_{n-2}(x)$ can be solved directly.

Improve accuracy with Newton’s method on original $P(x)$. 

Müller’s Method

- Similar to the Secant method, but parabola instead of line
- Fit quadratic polynomial $P(x) = a(x - p_2)^2 + b(x - p_2) + c$ that passes through $(p_0, f(p_0)), (p_1, f(p_1)), (p_2, f(p_2))$.
- Solve $P(x) = 0$ for $p_3$, choose root closest to $p_2$:
  \[
  p_3 = p_2 - \frac{2c}{b + \text{sgn}(b)\sqrt{b^2 - 4ac}}.
  \]
- Repeat until convergence
- Relatively insensitive to initial $p_0, p_1, p_2$, but e.g. $f(p_i) = f(p_{i+1}) = f(p_{i+2}) \neq 0$ gives problems