Week 4: NUMERICAL ANALYSIS
Solutions of Equations in One Variable

The Bisection Method

The Bisection Method

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

The Bisection Method – Implementation

MATLAB Code

```
function p=bisection(f,a,b,tol)

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
```

Bisection Method

Termination Criteria

- Many ways to decide when to stop:

$$
\begin{aligned}
|p_N - p_{N-1}| &< \varepsilon \\
\frac{|p_N - p_{N-1}|}{|p_N|} &< \varepsilon \\
|f(p_N)| &< \varepsilon
\end{aligned}
$$

- None is perfect, use a combination in real software

Convergence

Theorem

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*

$$|p_n - p| \leq \frac{b-a}{2^n}, \qquad \text{when } n \geq 1.$$

Convergence Rate

- The sequence $\{p_n\}_{n=1}^{\infty}$ converges to p with rate of convergence $O(1/2^n)$:

$$p_n = p + O\left(\frac{1}{2^n}\right).$$

Fixed Points

Fixed Points and Root-Finding

- 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:

$$g(x) = x - f(x)$$
$$g(x) = x + 3f(x)$$
$$\dots$$

- 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*

$$|g'(x)| \leq k, \qquad \text{for all } x \in (a, b),$$

then the fixed point in $[a, b]$ *is unique.*

Fixed-Point Iteration

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

```
function p=fixedpoint(g,p0,tol)

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

Convergence of Fixed-Point Iteration

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*

$$|g'(x)| \leq k, \qquad \text{for all } x \in (a, b).$$

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 $(p - p_0)^2$ neglibible:

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

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)

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.

Order of Convergence

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 λ and α 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* α, *with asymptotic error constant* λ.
An iterative technique $p_n = g(p_{n-1})$ is said to be of *order* α if the sequence $\{p_n\}_{n=0}^{\infty}$ converges to the solution $p = g(p)$ of order α.

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 ϕ giving $g'(p) = 0$ when $f(p) = 0$:

$$\begin{aligned} g'(x) &= 1 - \phi'(x)f(x) - f'(x)\phi(x) \\ g'(p) &= 1 - \phi'(p) \cdot 0 - f'(p)\phi(p) \end{aligned}$$

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

$$p_n = g(p_{n-1}) = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$$

Multiplicity of Zeros

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

$$0 = f(p) = f'(p) = f''(p) = \cdots = f^{(m-1)}(p), \text{ but } f^{(m)}(p) \neq 0.$$

Variants for Multiple Roots

Newton's Method for Multiple Roots

Define $\mu(x) = f(x)/f'(x)$. 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 μ. Newton's method can then be applied to μ to give

$$g(x) = x - \frac{f(x)f'(x)}{[f'(x)]^2 - f(x)f''(x)}$$

Aitken's Δ^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* Δp_n is defined by

$$\Delta p_n = p_{n+1} - p_n, \qquad \text{for } n \geq 0$$

Higher powers of the operator Δ are defined recursively by

$$\Delta^k p_n = \Delta(\Delta^{k-1} p_n), \qquad \text{for } k \geq 2$$

Aitken's Δ^2 method using delta notation

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

$$\hat{p}_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n}, \qquad \text{for } n \geq 0$$

Convergence of Aitken's Δ^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 Δ^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:

$$p_0^{(0)},\ p_1^{(0)} = g(p_0^{(0)}),\ p_2^{(0)} = g(p_1^{(0)}),\ p_0^{(1)} = \{\Delta^2\}(p_0^{(0)}),$$
$$p_1^{(1)} = g(p_0^{(1)}),\ \ldots$$

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 $p_0 \in [p-\delta, p+\delta]$.

Steffensen's Method

MATLAB Implementation

```
function p=steffensen(g,p0,tol)

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*

$$b_k = a_k + b_{k+1} x_0, \qquad \text{for } k = n-1, n-2, \ldots, 1, 0,$$

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

$$P'(x) = Q(x) + (x - x_0) Q'(x) \qquad \text{and} \qquad P'(x_0) = Q(x_0).$$

Horner's Method

MATLAB Implementation

```
function [y,z]=horner(a,x)

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);
```

Deflation

Deflation

- 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

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:

$$p_3 = p_2 - \frac{2c}{b + \operatorname{sgn}(b)\sqrt{b^2 - 4ac}}.$$

- 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