Lecture 3
Scientific and Data Computing I

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Model Components

• Cash Bond Model
  – $B(t)$ is the cash value at time $t$
  – $r$ is the rate-of-return (non-volatile).

• Fixed $r$:
  \[ B(t) = B(0) e^{rt} \]

• Variable $r(t)$:
  \[ B(t) = B(0) \exp \left( \int_0^t r(s) ds \right) \]
Profit Model

• Profit Model Assuming a Fixed Surcharge

\[ P(t) = B(t) - B(0) - C_0 \]

\[ P(t) = B(0) \cdot (e^{rt} - 1) - C_0 \]
Profit Model (Continued)

- Profit Versus Time Accounting for Surcharge
Root Finding Problem

- Bisection Method
- Newton’s Method
- Secant Method
Bisection Method

• Bisection Method (Algorithm)

Letting \( c_{i-1} = (a_{i-1} + b_{i-1})/2 \)
if \( f(c_{i-1}) = 0 \) then stop
else if \( f(a_{i-1})f(c_{i-1}) < 0 \) then \( a_i = a_{i-1}, b_i = c_{i-1} \)
else \( a_i = c_{i-1}, b_i = b_{i-1} \)

The error in the approximation satisfies \( |c_i - \bar{x}| \leq \frac{1}{2} \ell_i \)
Bisection Method (Continued)

• Why Bisect?

\[ \epsilon(\bar{c}) = |x^* - \bar{c}| \]
Bisection Method (Continued)

• On the theory side …

**Theorem 2.1** If \( f \in C[a, b] \), with \( f(a)f(b) < 0 \), then the midpoints \( c_0, c_1, c_2, \ldots \) computed using the bisection method converge to a solution \( \bar{x} \) of \( f(x) = 0 \), and the error satisfies

\[
|c_i - \bar{x}| \leq \frac{1}{2^{i+1}}(b - a)
\]
Additional Comments
  - Multiple Roots
  - Multi-dimensions

Classroom Demonstration in Matlab
Newton’s Method

• Newton’s Method (Algorithm)

\[ f(x) \approx f(x_0) + f'(x_0)(x - x_0) \]

Using the approximation and solving for \( x \):

\[ x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \]

\[ x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}, \text{ for } i = 0, 1, 2, 3, \ldots \]
Newton’s Method (Continued)

• Why does it work?
Newton’s Method (Continued)

• On the theory side …

**Theorem 2.2.** Assuming $f \in C^2(a, b)$, with $a < \bar{x} < b$ and $f'(x) \neq 0$ for $a < x < b$. In this case, for $x_0$ chosen close to the $\bar{x}$, Newton’s method will converge to $\bar{x}$. Moreover, if $f'''(\bar{x}) \neq 0$, and $x_0$ does not have the finite termination property, then

$$|x_{i+1} - \bar{x}| = C_i |x_i - \bar{x}|^2,$$

where, as $i \to \infty$,

$$C_i \to \left| \frac{f'''(\bar{x})}{2f'(\bar{x})} \right|$$
Higher-Order Extensions

• Halley’s Method:

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

• Re-written to “follow” Newton-method form:

\[x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \left[1 - \frac{f(x_n)}{f'(x_n)} \cdot \frac{f''(x_n)}{2f'(x_n)}\right]^{-1}\]
Issues In Practice

• Importance of the initial condition
• Runaway problem
• Zero slope problem

Classroom Demonstration in Matlab
Secant Method

- Secant Method Algorithm:

Approximate the derivative with:

\[ f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \]

\[ x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}, \text{ for } i = 1, 2, \ldots \]
Secant Method (Continued)

• On the theory side …

**Theorem 2.3.** Assuming $f \in C^2(a, b)$, with $a < \bar{x} < b$ and $f'(x) \neq 0$ for $a < x < b$. In this case, for $x_0$ and $x_1$ chosen close to the $\bar{x}$, the second method will converge to $\bar{x}$. Moreover, if $f''(\bar{x}) \neq 0$, and $x_0$ and $x_1$ does not have the finite termination property, then

$$|x_{i+1} - \bar{x}| = D_i |x_i - \bar{x}|^\gamma$$

where $\gamma = (1 + \sqrt{5})$, and as $i \to \infty$,

$$D_i \to \left| \frac{f''(\bar{x})}{2f'(\bar{x})} \right|^{-\frac{1}{\gamma}}$$
Issues In Practice

• Storage
• Multi-Dimensional Secant

Classroom Demonstration in Matlab
Automatic Differentiation

• Hand Differentiation
• Symbolic Differentiation
  – Symbolic Manipulation Software (Mathematica, Maple, etc.)
  – Translate to Code
• Numerical Differentiation
  – Finite Difference
  – Complex Step
• Automatic Differentiation
  – Analytically Differentiates Code Directly from Source
  – Preprocessor
  – Operator Overloading
For Next Time

• Read Chapter 2
• Look ahead to Chapter 7
• Start working on Practicums
• Start working on Homework 1