22S:166
Lecture 12
Oct. 6, 2008
Root-finding

Root finding algorithms

- problem: to find values of variable x that satisfy $f(x) = 0$ for given function f
- solution is called "zero of f" or "root of f"
- when is this an important problem in statistics?

The bisection method

- also called "binary-search method"
- conditions for use
  - f continuous, defined on interval $[a, b]$
  - $f(a)$ and $f(b)$ of opposite sign
- by Intermediate Value Theorem, there exists a $p,\ a < p < b$, such that $f(p) = 0$
- procedure works when $f(a)$ and $f(b)$ of opposite sign and more than one root in $[a, b]$
- for simplicity, we'll assume unique root in interval
- method consists of
  - repeated halving of subintervals of $[a, b]$
  - at each step, locating half containing p
- requires following inputs
  - endpoints a, b
  - tolerance TOL
  - maximum number of iterations N_0

Fixed-point iteration

- solution to
$$g(x) = x$$
is called *fixed point* of function g
- Theorem
  - conditions
    - g continuous on $[a, b]$
    - $g(x) \in [a, b]\ \forall x \in [a, b]$
  - conclusions
    - g has a fixed point in $[a, b]$
  - if further
    - $g'(x)$ exists on (a, b) and a positive constant $k < 1$ exists such that
$$|g'(x)| \le k < 1, \quad \forall x \in (a, b)$$
  - then
    - g has a unique fixed point p in $[a, b]$

Example 1

$$g(x) = \frac{x^2 - 1}{3} \text{ on } [-1, 1]$$

- absolute minimum of g is $g(0) = -\frac{1}{3}$
- absolute minimum of g is $g(\pm 1) = 0$
- $|g'(x)| = |\frac{2x}{3}| \leq \frac{2}{3} \;\; \forall x \in [-1, 1]$
- so g has unique fixed point p in interval
- in this case, can be determined exactly by quadratic formula

Example 2

$$g(x) = 3^{-x} \text{ on } [0, 1]$$

- $g(1) = \frac{1}{3} \leq g(x) \leq 1 = g(0) \; \forall \; 0 \leq x \leq 1$, so fixed point exists in interval
- theorem cannot be used to determine uniqueness of fixed point since $|g'(0)| = 1.0986 > 1$
- but fixed point must be unique since g is a decreasing function

Fixed-point iteration

- choose initial approximation p_0
- set $p_n = g(p_{n-1})$ for each $n \geq 1$

Example

$x^3 + 4x^2 - 10 = 0$ has unique root in $[1, 2]$.

Fixed-Point Theorem

- conditions
  - g continuous on on $[a, b]$
  - $g(x) \in [a, b] \; \forall x \in [a, b]$
  - $g'(x)$ exists on (a, b) and

$$|g'(x)| \leq k < 1, \quad \forall x \in (a, b)$$

- then if p_0 is any number in $[a, b]$ then the sequence defined by

$$p_n = g(p_{n-1}), \quad n \geq 1$$

  converges to the unique fixed point p in $[a, b]$

The Newton-Raphson Method

- one of most powerful and well-known numerical methods for solving root-finding problem $f(x) = 0$
- one derivation: Taylor series approximation
  - suppose f' and f'' are continuous on $[a, b]$
  - let $x_0 \in [a, b]$ be an approximation to p such that $f'(x_0) \neq 0$ and $|x_0 - p|$ is "small"
  - first order Taylor approximation for $f(x)$ expanded around x_0

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

    where $\xi(x)$ is between x and x_0.
  - with $x = p$ this gives

$$0 = f(x_0) + (p - x_0) f'(x_0) + \frac{(p - x_0)^2}{2} f''(\xi(x))$$

  - since $|x_0 - p|$ is "small", $(x_0 - p)^2$ should be negligible and

$$0 \simeq f(x_0) + (p - x_0) f'(x_0)$$

  - solving for p yields

$$p \simeq x_0 - \frac{f(x_0)}{f'(x_0)}$$

The Newton-Raphson Method

- start with initial approximation p_0
- let $p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}$

Convergence Theorem for Newton-Raphson Method

- conditions
  - f has continuous first and second derivatives on $[a, b]$
  - $p \in [a, b]$ is such that $f(p) = 0$ and $f'(p) \neq 0$
- conclusions
  - 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 $p_0 \in [p - \delta, p + \delta]$.

The Secant Algorithm

- useful when computation of $f'(x)$ is far more computationally intensive than computation of $f(x)$
- uses forward (or backward)-difference formula to approximate $f'(p_{n-1})$

$$f'(p_{n-1}) \simeq \frac{f(p_{n-2}) - f(p_{n-1})}{p_{n-2} - p_{n-1}} = \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}$$

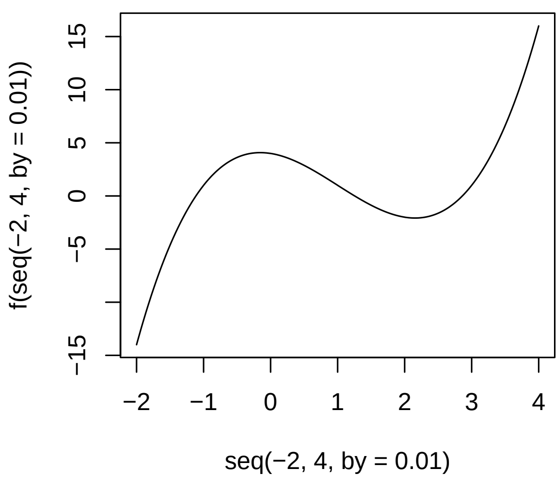
- Secant algorithm generates sequence as

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}, \; n \geq 1$$

uniroot function in R

```
uniroot                package:stats                R Documentation

One Dimensional Root (Zero) Finding

Description:

     The function 'uniroot' searches the interval from 'lower' to
     'upper' for a root (i.e., zero) of the function 'f' with respect
     to its first argument.

Usage:

     uniroot(f, interval, lower = min(interval), upper = max(interval),
             tol = .Machine$double.eps^0.25, maxiter = 1000, ...)
```


Example




```
> f <- function(x) {x^3 - 3*x^2 -x + 4}
> plot(seq(-2,4,by=0.01), f(seq(-2,4,by=0.01)),type="l")
> uniroot(f=f,c(-2,4))
$root
[1] -1.114907

$f.root
[1] 9.607438e-06

$iter
[1] 9

$estim.prec
[1] 6.103516e-05
```