Informatics

Numerical Methods

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Learning Objectives

- Show some solutions of mathematical problems through computation, instead of analytics
- see the `numerical_methods` folder on GitHub

Finding the root of a function

find x such that f(x) = 0

Finding the root with the Newton method

- let f(x) have the derivative f'(x)
- based on the Taylor approximation
- convergence is not guaranteed in general

$$
\begin{aligned}
x_0 &= \qquad \text{initial guess} \\
x_n &= \quad x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}
\end{aligned}
$$

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

see example **`newton.R`**

Zero of a function with the *bisection* algorithm

- start with two values such that f(x1)*f(x2) < 0
  - the sign is opposite
- if f is continuous the zero will lie somewhere between x1 and x2
- choose the midpoint x between x1 and x2
- choose the next interval accordingly to the sign of f(x)
- stop looping when a pre-set precision is met

see example **`bisect.R`**

Finding the minimum of a function

- analytic solutions are based on the derivative of the function
- it happens that a function is not differentiable in the interval of interest
- the minimum can be found by search
- the quality of the solution is related to
  - precision
  - convergence speed
- necessary a strategy to choose the test points

Golden Section search method

Braun, Murdoch, "Statistical programming with R", Cambridge

- valid for a function that has a single minimum on a given interval [a,b]
- iterative solution
  - based on a loop that ends when a given stop condition is met

1. start with the interval that is known to contain the minimizer
2. repeatedly shrink it, finding smaller and smaller intervals [a',b'] which contain the minimizer
3. stop when b'-a' is small enough, i.e. when the interval length is less than a pre-set *tolerance*
4. use as minimizer the midpoint of the last interval
5. the maximum error is (b'-a')/2

Golden Section Search (ii)

- Let's name x1 and x2 the points where we will test the function
- in step 2 we choose $x1 < x2$
  - we will see how in a short while
- if $f(x1) > f(x2)$ the minimizer must lie to the right of x1
  - new interval $[a',b'] = [x1,b]$
- if $f(x1) < f(x2)$ the minimizer must lie to the left of x2
  - new interval $[a',b'] = [a,x2]$
- if they are equal simply choose always one side
- choose new values x1 and x2 and compute the function in the chosen points, until the stop condition is met

The Golden Ratio

Golden ratio ≅ 0.618
therefore x1 < x2

- interesting algebraic properties

$$\phi = (\sqrt{5}+1)/2$$
$$1/\phi = \phi - 1$$
$$1/\phi^2 = 1 - 1/\phi$$

$$x_1 = b - (b-a)/\phi$$
$$x_2 = a + (b-a)/\phi$$

Golden Ratio Search

- after one iteration it is possible that we throw away a and replace it with a' = x1
- new value to use as x1 ➞
- i.e., we can re-use a point already used, without need of a new calculation

$$\begin{aligned} x_1' &= b - (b - a')/\phi \\ &= b - (b - x_1)/\phi \\ &= b - (b - a)/\phi^2 \\ &= a + (b - a)/\phi \\ &= x_2 \end{aligned}$$

see example **`golden_search.R`**