MATH-458 Programming Concepts in Scientific Computing: Nonlinear Solvers

Michael Jaquier Alexander Lorkowski

1 Introduction

2 Algorithm

2.1 Bisection Method

The bisection method is based on Theorem 1.

Theorem 1. *(Zeros of a continuous functions)*
Given a continuous function f : [a,b] → R, such that f(a)f(b) < 0, then ∃ at least an α ⊂ (a,b) such that f(α) = 0.

Starting from I_0 = [a,b], the bisection method generates a sequence of subintervals I_k = [a(k),b(k)], k ≥ 0, with $I_k \subset I_k 1$, k ≥ 1, and enjoys the property that f(a(k))f(b(k)) < 0.

Algorithm 1 Bisection Method

$k \leftarrow 0$, $a^{(0)} \leftarrow$ a, $b^{(0)} \leftarrow$ b, $x^{(0)} \leftarrow (a^{(0)}+b^{(0)})/2$
while $x^{(k)} >$ tol and k < k_{max} **do**
  if f($x^{(k-1)}$) == 0 **then return** $\alpha = x^{(k-1)}$
  else
    if f($x^{(k-1)}$)f($a^{(k-1)}$) < 0 **then**
      set $a^{(k)} = a^{(k-1)}$ and $b^{(k)} = x^{(k-1)}$
    if f($x^{(k-1)}$)f($b^{(k-1)}$) < 0 **then**
      set $a^{(k)} = x^{(k-1)}$ and $b^{(k)} = b^{(k-1)}$
    set $x^{(k)} = (a^{(k)}+b^{(k)})/2$
return $\alpha = x^{(k)}$

2.2 Newton/Quasi-Newton Methods

Assuming that f ⊂ $C^0(I)$ and is differentiable in the interval I = (a,b) ⊆ R, the equation of a tangenet line to the curve $(x, f(x))$ at coordinate $x^{(k)}$, where $x^{(k)} \subset$ I, is y(x) = f($x^{(k)}$)+df($x^{(k)}$)(x - $x^{(k)}$). If we assume y($x^{(k)}$) = 0, $x^{(k+1)}$ can be computed from Eq. 1.

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{q^{(k)}} \tag{1}$$

with $q^{(k)}$ determining the method as Newton (Eq. 2) or Chord (Eq. 3):

$$q^{(k)} = \frac{df(x^{(k)})}{dx} \tag{2}$$

$$q^{(k)} = \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}} \tag{3}$$

Algorithm 2 General quasi-Newton Method

1: $k \leftarrow 0$, set initial guess $x^{(0)}$
2: **while** $x^{(k)} >$ tol and k < k_{max} **do**
3: $x^{(k+1)} = x^{(k)}$ - $\frac{f(x^{(k)})}{(q^{(k)}}$
4: k = k + 1;
return $\alpha = x^{(k)}$

2.3 Fixed Point Iteration

For a given f : [a,b] $\rightarrow$ R, the problem can be transformed from f(x) = 0 into an equivalent problem x - ϕ(x) = 0. The auxiliary function ϕ : [a,b] $\rightarrow$ R has to chosen in such a way that $\phi(\alpha) = \alpha$ whenever f(α) = 0. Finding the fixed points of the mapping ϕ thus results in finding the roots of the original equation f(x), hence the name fixed point iteration.

Algorithm 3 Fixed point iterations

1: $k \leftarrow 0$, set initial guess $x^{(0)}$
2: **while** $x^{(k)}$ - $x^{(k-1)} >$ tol and k < k_{max} **do**
3: $x^{(k+1)} = \phi(x^{(k)})$
4: k = k + 1;
return $\alpha = x^{(k)}$

2.4 Aitken Method

Aitkens method provides a way to accelerate the convergence of iterative methods for finding the roots of a function. The general algorithm is shown below.

Algorithm 4 Aitken Method

1: $k \leftarrow 0$, set initial guess $x^{(0)}$
2: **while** $x^{(k)}$ - $x^{(k-1)} >$ tol and k < k_{max} **do**
3: Calculate x_{3i+1} and x_{3i+2} using any linear iterative method.
4: Modify x_{3i+2} using $x_{3i+2} = x_{3i}$ - $\frac{(x_{3i+1}-x_{3i})^2}{(x_{3i}-2*x_{3i+1}+x_{2i+2})}$
5: k = k + 1;
return $\alpha = x^{(k)}$

3 Program Structure