Computational Science:
Computational Methods in Engineering

Single Variable Optimization

Outline

- Mathematical Preliminaries
- Single Variable Optimization
  - Parabolic interpolation
  - Newton's method

Mathematical Preliminaries

3

Recall Derivative Tests

First-order derivatives convey slope and whether the function is at an extremum or not.

The sign of second-order derivatives convey whether the extremum is a minimum or a maximum.

EMPossible

4

Parabolic Interpolation

Formulation of the Method

Fit $f(x)$ to a polynomial and then use the first-derivative test to find the extremum.

Step 1 – Pick three points that span an extremum

x_1 and $f_1 = f(x_1)$ $\quad$ x_2 and $f_2 = f(x_2)$ $\quad$ x_3 and $f_3 = f(x_3)$

Step 2 – Fit the points to a polynomial

$$f(x) \approx a_0 + a_1 x + a_2 x^2 \qquad \begin{matrix} f_1 \approx a_0 + a_1 x_1 + a_2 x_1^2 \\ f_2 \approx a_0 + a_1 x_2 + a_2 x_2^2 \\ f_3 \approx a_0 + a_1 x_3 + a_2 x_3^2 \end{matrix} \Rightarrow \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} \Rightarrow \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix}^{-1} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

Step 3 – Use the first derivative test to find the extremum

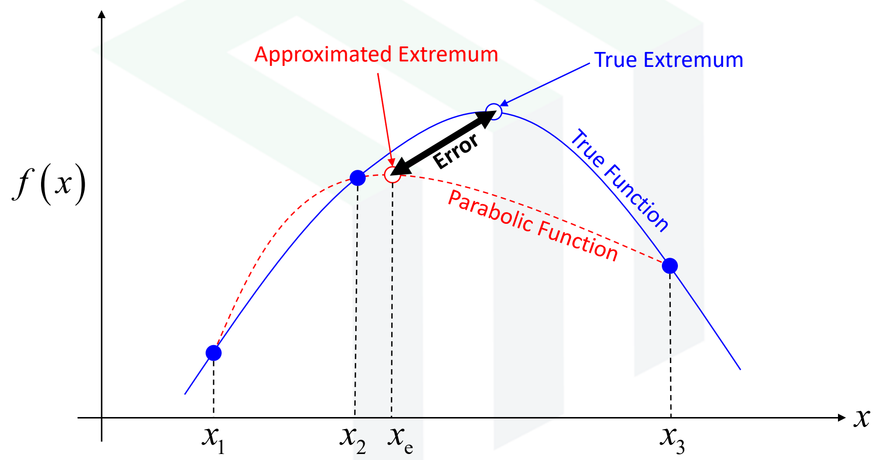
$$f'(x) \approx a_1 + 2a_2 x \;\rightarrow\; f'(x_e) \approx a_1 + 2a_2 x_e = 0 \;\rightarrow\; x_e = -\frac{a_1}{2a_2}$$

Step 4 – After working through the algebra, the final expression for the extremum is

$$x_e = \frac{1}{2} \frac{f(x_1)(x_2^2 - x_3^2) + f(x_2)(x_3^2 - x_1^2) + f(x_3)(x_1^2 - x_2^2)}{f(x_1)(x_2 - x_3) + f(x_2)(x_3 - x_1) + f(x_3)(x_1 - x_2)}$$

EMPossible

Visualization of the Method



EMPossible

7

Newton's Method

8

Formulation of the Method

Recall that the Newton-Raphson method was used to find the zero of a function. Starting with an initial guess x_i for the root, the following equation was iterated until convergence.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

This is easily converted into an algorithm for finding an extremum instead of a zero. Define an auxiliary function $g(x)$ that is the first derivative of $f(x)$.

$$g(x) = \frac{df(x)}{dx} = f'(x)$$

The auxiliary function $g(x)$ will have a zero at an extremum of $f(x)$. This means the Newton-Raphson method can be performed on $g(x)$ to find an extremum of $f(x)$.

$$g(x) = \frac{df(x)}{dx} = f'(x) \quad \Rightarrow \quad x_{i+1} = x_i - \frac{g(x_i)}{g'(x_i)}$$

EMPossible

9