Computational Science:
Computational Methods in Engineering

Single Variable Optimization

Outline

• Mathematical Preliminaries
• Single Variable Optimization
  • Parabolic interpolation
  • Newton’s method
  • Golden-section search
Mathematical Preliminaries

Recall Derivative Tests

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

\[ f'' = 0 \]

- \( f' > 0 \) \( \rightarrow \) maximum
- \( f' < 0 \) \( \rightarrow \) minimum
- \( f' = 0 \)

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

\[ f'' > 0 \]

- maximum

\[ f'' < 0 \]

- minimum
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

$x_i$ and $f_i = f(x_i)$ and $x_j = f(x_j)$ and $f_k = f(x_k)$

Step 2 – Fit the points to a polynomial

\[ f(x) = a_0 + a_1 x + a_2 x^2 \]

\[
\begin{bmatrix}
  f_i \\
  f_j \\
  f_k
\end{bmatrix} = \begin{bmatrix}
  x_i^2 & x_i & 1 \\
  x_j^2 & x_j & 1 \\
  x_k^2 & x_k & 1
\end{bmatrix} \begin{bmatrix}
  a_0 \\
  a_1 \\
  a_2
\end{bmatrix}
\]

Step 3 – Use the first derivative test to find extremum

\[ f'(x) = a_1 + 2a_2 x \quad \Rightarrow \quad f'(x) = a_1 + 2a_2 x = 0 \quad \Rightarrow \quad x = -\frac{a_1}{2a_2} \]

Step 4 – After working through the algebra, we get a final expression for the extremum

\[ x_e = \frac{1}{2} \frac{f(x_i)(x_j^2 - x_i^2) + f(x_j)(x_k^2 - x_j^2) + f(x_k)(x_i^2 - x_k^2)}{f(x_i)(x_j - x_i) + f(x_j)(x_k - x_j) + f(x_k)(x_i - x_k)} \]
Visualization of the Method

![Graph showing visualization of the method]

Newton’s Method
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.

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

We can easily convert this 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 we can perform the Newton-Raphson method on $g(x)$ to find an extremum of $f(x)$.

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

Golden Section Search
Step 1 – Define Interval

Pick lower and upper limits, $x_L$ and $x_U$, so that $f(x)$ has only one extremum inside the interval.

Step 2 – Evaluate the Function at the Bounds

$$f_L = f(x_L) \quad f_U = f(x_U)$$
Step 3 – Pick Two Intermediate Points $x_1$ and $x_2$

$$x_1 = x_U - d \quad x_2 = x_L + d$$

$$d = R(x_U - x_L) \quad R = \frac{\sqrt{5} - 1}{2} \approx 0.6180...$$

Step 4 – Evaluate the Function at Points $x_1$ and $x_2$

$$f_1 = f(x_1) \quad f_2 = f(x_2)$$
Step 5a – Determine the Position of the Maximum

If $f_1 > f_2$, then the maximum is on the left side of the interval between $x_L$ and $x_2$.
If $f_1 < f_2$, then the maximum is on the right side of the interval between $x_1$ and $x_U$.

Step 5b – Adjust Points

$x_L = x_1$, $x_1 = x_2$, $x_2 = x_L + R(x_U - x_L)$, $f_2 = f(x_2)$
Step 5c – Determine the Position of the Maximum

If \( f_1 > f_2 \), then the maximum is on the left side of the interval between \( x_L \) and \( x_2 \).
If \( f_1 < f_2 \), then the maximum is on the right side of the interval between \( x_1 \) and \( x_U \).

Step 5b – Adjust Points

\[
\begin{align*}
    x_U &= x_2 \\
    f_U &= f_2 \\
    x_2 &= x_1 \\
    f_2 &= f_1 \\
    x_1 &= x_U - R(x_U - x_L) \\
    f_1 &= f(x_1)
\end{align*}
\]
Step 5c – Repeat Until Convergence

Converged if:
\[ 2 \frac{|x_U - x_L|}{x_U + x_L} < \text{tolerance} \]

Step 6 – Calculate Final Answer

Estimate the final extremum to be at the midpoint of the last interval.

\[ x_e \approx \frac{x_U + x_L}{2} \]
Algorithm Summary for Finding a Maximum

1. Define starting bounds \( x_L \) and \( x_U \).
   \[ \frac{x_L}{x_U} \leq x \leq \frac{x_U}{x_L} \]
2. Evaluate the function at the two bounding points.
   \[ f_L = f(x_L) \quad f_U = f(x_U) \]
3. Pick two intermediate points, \( x_1 \) and \( x_2 \), using Golden ratio.
   \[ R = \frac{\sqrt{5} - 1}{2} \approx 0.618033988749895... \]
   \[ x_1 = x_U - R(x_U - x_L) \]
   \[ x_2 = x_L + R(x_U - x_L) \]
4. Evaluate function at the two intermediate points.
   \[ f_1 = f(x_1) \quad f_2 = f(x_2) \]
5. Update bounds by identifying position of the maximum.
   If \( f_1 > f_2 \), maximum is on left side.
   \[ x_L = x_1 \quad f_L = f_1 \]
   \[ x_U = x_2 \quad f_U = f_2 \]
   \[ x_i = x_U - R(x_U - x_L) \quad f_i = f(x_i) \]
   If \( f_1 < f_2 \), maximum is on right side.
   \[ x_L = x_1 \quad f_L = f_1 \]
   \[ x_U = x_2 \quad f_U = f_2 \]
   \[ x_i = x_L + R(x_U - x_L) \quad f_i = f(x_i) \]
6. Repeat Step 5 until convergence
   \[ \frac{x_U - x_L}{x_U + x_L} < \text{tolerance} \]
7. Calculate final answer
   \[ x = \frac{x_U + x_L}{2} \quad f_s = f(x_s) \]

Algorithm Summary for Finding a Minimum

1. Define starting bounds \( x_L \) and \( x_U \).
   \[ \frac{x_L}{x_U} \leq x \leq \frac{x_U}{x_L} \]
2. Evaluate the function at the two bounding points.
   \[ f_L = f(x_L) \quad f_U = f(x_U) \]
3. Pick two intermediate points, \( x_1 \) and \( x_2 \), using Golden ratio.
   \[ R = \frac{\sqrt{5} - 1}{2} \approx 0.618033988749895... \]
   \[ x_1 = x_U - R(x_U - x_L) \]
   \[ x_2 = x_L + R(x_U - x_L) \]
4. Evaluate function at the two intermediate points.
   \[ f_1 = f(x_1) \quad f_2 = f(x_2) \]
5. Update bounds by identifying position of the minimum.
   If \( f_1 < f_2 \), minimum is on left side.
   \[ x_L = x_1 \quad f_L = f_1 \]
   \[ x_U = x_2 \quad f_U = f_2 \]
   \[ x_i = x_U - R(x_U - x_L) \quad f_i = f(x_i) \]
   If \( f_1 > f_2 \), minimum is on right side.
   \[ x_L = x_1 \quad f_L = f_1 \]
   \[ x_U = x_2 \quad f_U = f_2 \]
   \[ x_i = x_L + R(x_U - x_L) \quad f_i = f(x_i) \]
6. Repeat Step 5 until convergence
   \[ \frac{x_U - x_L}{x_U + x_L} < \text{tolerance} \]
7. Calculate final answer
   \[ x = \frac{x_U + x_L}{2} \quad f_s = f(x_s) \]
Animation of the Method

Derivation of Golden Ratio (1 of 2)

From this picture, define three length parameters.

\[ \ell_0 = x_0 - x_L \]
\[ \ell_1 = x_1 - x_L \]
\[ \ell_2 = x_U - x_2 \]

Recognizing that the points of the next iteration should lie on top of points from the previous iteration, define two conditions to ensure this.

\[ \ell_0 = \ell_1 + \ell_2 \]  
**Condition 1** – ensures \( \ell_1 + \ell_2 \) covers entire span.

\[ \frac{\ell_1}{\ell_0} = \frac{\ell_2}{\ell_1} \]  
**Condition 2** – ensures the next iteration has the same proportional spacing as the current iteration.
Derivation of Golden Ratio (2 of 2)

\[ \ell_0 = \ell_1 + \ell_2 \] 
Condition 1 – ensures \( \ell_1 + \ell_2 \) covers entire span.

\[ \ell_1 = \ell_2 \] 
Condition 2 – ensures the next iteration has the same proportional spacing as the current iteration.

Substitute Condition 1 into Condition 2 to eliminate \( \ell_0 \).

\[ \frac{\ell_1}{\ell_1 + \ell_2} = \frac{\ell_2}{\ell_2} \]

Define the Golden ratio as \( R = \frac{\ell_2}{\ell_1} \).

\[ \frac{\ell_1}{\ell_1 + \ell_2} = \frac{\ell_2}{\ell_1} \quad \rightarrow \quad \frac{\ell_1 + \ell_2}{\ell_1} = \frac{\ell_1}{\ell_2} \quad \rightarrow \quad 1 + \frac{\ell_2}{\ell_1} = \frac{\ell_1}{\ell_2} \quad \rightarrow \quad 1 + \frac{1}{R} = \frac{1}{R} \quad \rightarrow \quad R^2 + R - 1 = 0 \]

Solve for \( R \) using the quadratic formula.

\[ R = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \rightarrow \quad -1 \pm \sqrt{5} \quad \rightarrow \quad R = \frac{-1 + \sqrt{5}}{2} \]

Pick the positive root to keep \( R \) positive.

\[ R = \frac{\sqrt{5} - 1}{2} \approx 0.618033988749895... \]

The Magic of the Golden-Section Search

Three of the four points line up from one iteration to the next. This means the function only has to be evaluated at one new point each iteration.

The interval is reduced by 38.2% each iteration.