Numerical Analysis

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Fibonacci Search

Assume $f : [a, b] \to \mathbb{R}$ is unimodal and continuous on interval $[a, b]$.

Without any evaluation of function f we can take the midpoint $\hat{x}$ of $[a, b]$ as approximation of the minimum point x^* and in that case

$$|\hat{x} - x^*| \leq \frac{b-a}{2}.$$

If we evaluate f at one point, again the best we can do is to take the midpoint $\hat{x}$ as an approximation of x^*.

Assume f is evaluated at two points A and B.

If $f(A) > f(B)$ then $x^* \in [A, b]$.

If $f(A) \leq f(B)$ then $x^* \in [a, B]$.

Let's take

$$A = \frac{b+a}{2} - \delta,$$

$$B = \frac{b+a}{2} + \delta.$$

Then we take the midpoint $\hat{x}$ of appropriate subinterval $[A, b]$ or $[a, B]$ as approximation of x^* and

$$|\hat{x} - x^*| \leq \frac{b-a}{4} + \frac{\delta}{2}.$$

Assume f is evaluated at three points.

$$A = a + \frac{b-a}{3},$$

$$B = b - \frac{b-a}{3}.$$

If $f(A) > f(B)$ then $x^* \in [A, b]$.

If $f(A) \leq f(B)$ then $x^* \in [a, B]$.

Assume $x^* \in [A, b]$

Next evaluation is made at $B + \delta$.

If $f(B) > f(B + \delta)$ then $x^* \in [B, b]$. We take as approximation the midpoint of $[B, b]$ and

$$|\hat{x} - x^*| \leq \frac{b - a}{6}.$$

If $f(B) \leq f(B + \delta)$ then $x^* \in [a, B + \delta]$. We take as approximation the midpoint of $[a, B + \delta]$ and

$$|\hat{x} - x^*| \leq \frac{b - a}{6} + \frac{\delta}{2}.$$

Fibonacci Sequence

$$F_0 = 1, \qquad F_1 = 1,$$

$$F_k = F_{k-1} + F_{k-2}, \quad k \geq 2.$$

By continuing the search pattern outlined, we find an estimate $\hat{x}$ with only n evaluations of f and with an error

$$|\hat{x} - x^*| \leq \frac{b-a}{2F_n} + \frac{\delta}{2}.$$

Let's denote $[a_0, b_0] = [a, b]$.

$$\gamma_0 = \frac{F_{n-2}}{F_n}, \quad n \geq 3.$$

$$A_0 = a_0 + \gamma_0(b_0 - a_0)$$
$$B_0 = b_0 - \gamma_0(b_0 - a_0)$$

$$[a_1, b_1] = \begin{cases} [a_0, B_0], & \text{if } f(A_0) < f(B_0), \\ [A_0, b_0], & \text{if } f(A_0) \geq f(B_0). \end{cases}$$

$$x^* \in [a_1, b_1]$$

$$b_1 - a_1 = \frac{F_{n-1}}{F_n}(b - a)$$

$$\gamma_1 = \frac{F_{n-3}}{F_{n-1}}$$

$$A_1 = a_1 + \gamma_1(b_1 - a_1)$$
$$B_1 = b_1 - \gamma_1(b_1 - a_1)$$

If $[a_1, b_1] = [a_0, B_0]$, $B_1 = A_0$.
If $[a_1, b_1] = [A_0, b_0]$, $A_1 = B_0$.

$$\gamma_k = \frac{F_{n-2-k}}{F_{n-k}}, \quad k = 0, 1, \ldots, n-3.$$

$$A_k = a_k + \gamma_k(b_k - a_k)$$
$$B_k = b_k - \gamma_k(b_k - a_k)$$

$$[a_{k+1}, b_{k+1}] = \begin{cases} [a_k, B_k], & \text{if } f(A_k) < f(B_k), \\ [A_k, b_k], & \text{if } f(A_k) \geq f(B_k). \end{cases}$$

$$x^* \in [a_{k+1}, b_{k+1}]$$

$$b_{k+1} - a_{k+1} = \frac{F_{n-1-k}}{F_n}(b - a)$$

At the end of step $k = n - 3$ we have an interval $[a_{n-2}, b_{n-2}]$ with a length of $b_{n-2} - a_{n-2} = \frac{2}{F_n}(b - a)$. At this step we made $n - 1$ evaluations.

Then we need to evaluate f at a point δ away from the midpoint of $[a_{n-2}, b_{n-2}]$.

As approximation we take the midpoint of final interval.

Bisection Method

Assume $f : [a, b] \to \mathbb{R}$ is a unimodal and continuously differentiable function on $[a, b]$ and $f'(a)f'(b) < 0$.

Let's denote

$$[a_0, b_0] = [a, b]$$

and

$$x_0 = \frac{a_0 + b_0}{2}.$$

If $f'(x_0) = 0$, then we stop here.

$$[a_1, b_1] = \begin{cases} [a_0, x_0], & \text{if} \quad f'(x_0) > 0, \\ [x_0, b_0], & \text{if} \quad f'(x_0) < 0. \end{cases}$$

n-th step

$$[a_n, b_n] = \begin{cases} [a_{n-1}, x_{n-1}], & \text{if} \quad f'(x_{n-1}) > 0, \\ [x_{n-1}, b_{n-1}], & \text{if} \quad f'(x_{n-1}) < 0. \end{cases}$$

$$x_n = \frac{a_n + b_n}{2}.$$

If at n-th step $f'(x_n) = 0$, then we terminate our search.

Stopping conditions for the Bisection Method

- $|x_n - x_{n-1}| < \varepsilon$ or $\frac{|x_n - x_{n-1}|}{|x_{n-1}|} < \varepsilon$, if $x_{n-1} \neq 0$
- $|f'(x_n)| < \varepsilon$
- $|f(x_n) - f(x_{n-1})| < \varepsilon$ or $\frac{|f(x_n) - f(x_{n-1})|}{|f(x_{n-1})|} < \varepsilon$, if $f(x_{n-1}) \neq 0$

Example

Calculate the second approximation x_2 of the bisection method for the function $f(x) = -\frac{x^3}{3} + 2x$ on the interval $[-4, 0]$.

Newton's Method

Assume $f : \mathbb{R} \to \mathbb{R}$ is a twice differentiable function on $\mathbb{R}$.

Let x_0 be the initial approximation of the minimum point. Then we construct a quadratic function that matches its first and second derivatives at x_0 with that of the function f. This quadratic function has the form

$$q(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2.$$

Then, instead of minimizing f, we minimize its approximation q.

The first-order necessary condition for a minimizer of q yields

$$0 = q'(x) = f'(x_0) + f''(x_0)(x - x_0).$$

The solution of this equation will be the next approximation

$$x_1 = x_0 - \frac{f'(x_0)}{f''(x_0)}.$$

Reapplying this procedure we get the sequence defined by Newton's Method

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}, k = 1, 2, \ldots.$$

Stopping conditions

- $|x_n - x_{n-1}| < \varepsilon$ or $\frac{|x_n - x_{n-1}|}{|x_{n-1}|} < \varepsilon$, if $x_{n-1} \neq 0$
- $|f'(x_n)| < \varepsilon$
- $|f(x_n) - f(x_{n-1})| < \varepsilon$ or $\frac{|f(x_n) - f(x_{n-1})|}{|f(x_{n-1})|} < \varepsilon$, if $f(x_{n-1}) \neq 0$

Multivariate Case

Gradient Methods

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable function that we wish to minimize.

Let's denote by $\nabla f(x)$ the gradient of f at x, i.e.,

$$\nabla f(x) = \left[\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x), \ldots, \frac{\partial f}{\partial x_n}(x)\right]^T$$

Example

Let $f : \mathbb{R}^3 \to \mathbb{R}$ be defined by $f(x_1, x_2, x_3) = x_1^3 + 4x_2^2 x_1 + \sin(x_3^2 x_2)$. Compute the gradient $\nabla f(x_1, x_2, x_3)$.

Example

Let $f : \mathbb{R}^n \to \mathbb{R}$ be defined $f(x) = a^T x$, where $a \in \mathbb{R}^n$. Compute the gradient $\nabla f(x)$.

Here we consider algorithms of the form

$$x^{(k+1)} = x^{(k)} + \alpha_k d^{(k)}, \quad k = 0, 1, \dots,$$

where x_0 is the initial approximation,

$$d^{(k)} = -\frac{\nabla f\left(x^{(k)}\right)}{||\nabla f\left(x^{(k)}\right)||}$$

and $\alpha_k \geq 0$ is the step size.

The Steepest Descent Method

Assume x_0 is the initial approximation. The Steepest Descent Method is a gradient algorithm

$$x^{(k+1)} = x^{(k)} - \alpha_k \nabla f\left(x^{(k)}\right), \quad k = 0, 1, \dots,$$

where α_k is chosen to be the global minimizer of $\Phi_k(\alpha)$

$$\alpha_k = \text{arg min}_{\alpha \geq 0} \Phi_k(\alpha) = \text{arg min}_{\alpha \geq 0} f\left(x^{(k)} - \alpha \nabla f(x^{(k)}\right).$$

Stopping conditions

- $||\nabla f\left(x^{(k)}\right)|| < \varepsilon$
- $||x^{(k+1)} - x^{(k)}|| < \varepsilon$ or $\frac{||x^{(k+1)}-x^{(k)}||}{||x^{(k)}||} < \varepsilon$ if $||x^{(k)}|| \neq 0$
- $\left|f\left(x^{(k+1)}\right) - f\left(x^{(k)}\right)\right| < \varepsilon$ or $\frac{\left|f\left(x^{(k+1)}\right)-f\left(x^{(k)}\right)\right|}{\left|f\left(x^{(k)}\right)\right|} < \varepsilon$ if $f\left(x^{(k)}\right) \neq 0$.

Example

Assume we want to use the Steepest Descent Method to minimize

$$f(x_1, x_2) = 2x_1^2 + x_2^2.$$

We start with $x^{(0)} = (1, 2)^T$. Calculate $x^{(2)} = \left(x_1^{(2)}, x_2^{(2)}\right)^T$ by using the Steepest Descent Method.

Example

Assume we want to use the Steepest Descent Method to minimize

$$f(x_1, x_2) = x_1^2 + x_2^2.$$

We start with $x^{(0)} = (1, 2)^T$. Calculate $x^{(1)} = \left(x_1^{(1)}, x_2^{(1)}\right)^T$ by using the Steepest Descent Method.