Deterministic Optimization

Unconstrained Optimization: Derivative-Free Methods

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Univariate functions

Optimality Conditions

Learning objectives:

- Examine Golden section and Quadratic Fit methods

Derivative-free Algorithms for Unconstrained Optimization

$$(P): \quad \min\{f(x) \mid x \in \mathbb{R}^n\}.$$

- Golden Section search $(n = 1)$
- Quadratic fit $(n = 1)$
- Nelder-Mead method $(n > 1)$

Golden Section Search

Start with an initial interval $[x_l, x_u]$ containing the minima, and successively narrow this interval.

Step 0: Set $x_1 = x_u - \alpha(x_u - x_l)$ and $x_2 = x_l + \alpha(x_u - x_l)$. Compute $f(x)$ at x_l, x_1, x_2, x_u.

Step 1: If $(x_u - x_l) \leq \varepsilon$ stop and return $x^* = 0.5(x_l + x_u)$ as the minima.

Golden Section Search

Step 2: If $f(x_1) < f(x_2)$ set $x_u \leftarrow x_2$, $x_2 \leftarrow x_1$, and $x_1 \leftarrow x_u - \alpha(x_u - x_l)$. Evaluate $f(x_1)$.

Else set $x_l \leftarrow x_1$, $x_1 \leftarrow x_2$, and $x_2 \leftarrow x_l + \alpha(x_u - x_l)$. Evaluate $f(x_2)$.

Goto Step 1.

Requires one function evaluation per iteration.

Use $\alpha = 0.618$ the "Golden Ratio."

Quadratic Fit

- Let $x_m \in (x_l, x_u)$ such that $f(x_m) \leq f(x_l)$ and $f(x_m) \leq f(x_u)$.

- Approximate $f(x)$ by a quadratic

$$q(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2$$

  The coefficients are solutions the linear system obtained by setting $q(x_i) = f(x_i)$ for $i \in \{l, m, u\}$.

- Note that $q(x)$ is minimized at $x_q = \frac{-\alpha_1}{2\alpha_2}$.

Quadratic Fit

- By some tedious algebra

$$x_q = \frac{1}{2}\frac{f_l[x_m^2 - x_u^2] + f_m[x_u^2 - x_l^2] + f_u[x_l^2 - x_m^2]}{f_l[x_m - x_u] + f_m[x_u - x_l] + f_u[x_l - x_m]},$$

where $f_i = f(x_i)\ i \in \{l, m, u\}$.

Quadratic Fit

Step 0: Choose x_l, x_m, x_u. Let ϵ be a termination tolerance.

Step 1: If $(x_u - x_l) \leq \epsilon$ stop and return x_m as the minima.

Step 2: Compute x_q. If $x_q \approx x_m$ go to Step 3; if $x_q < x_m$ go to Step 4; if $x_q > x_m$ go to Step 5.

Quadratic Fit

Step 3: If $(x_m - x_l) > (x_u - x_m)$ then $x_q \leftarrow x_m - 0.5\epsilon$ and go to Step 4; else $x_q \leftarrow x_m + 0.5\epsilon$ and go to Step 5.

Step 4: If $f(x_m) < f(x_q)$ then $x_l \leftarrow x_q$; otherwise $x_u \leftarrow x_m$ and $x_m \leftarrow x_q$. Go to Step 1.

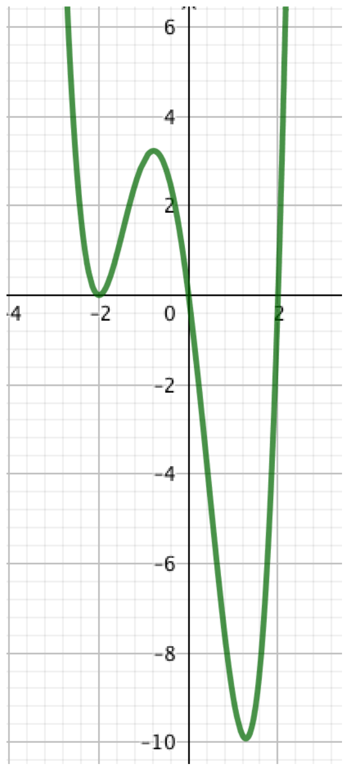
Step 5: If $f(x_m) < f(x_q)$ then $x_u \leftarrow x_q$; otherwise $x_l \leftarrow x_m$ and $x_m \leftarrow x_q$. Go to Step 1.

The MATLAB routine `fminbnd` uses a combination of Golden section and Quadratic search.

See also the routines in `scipy.optimize` (`www.scipy.org`)

Quadratic Fit

```
>>>
>>>
>>> from scipy.optimize import minimize_scalar
>>> def f(x):
...     return (x-2)*x*(x+2)**2
...
>>> res = minimize_scalar(f,bounds=(0,2),method='Golden')
>>> res.x
1.280776401465682
>>>
```



Summary

- Derivative free methods use only function evaluations to bracket a local minimum point
- Two example methods are Golden section and Quadratic fit