MATH 612: CM4ES&FM

Spring'14

Work'n'code time

May 12

The Nelder-Mead algorithm

We are going to code the Nelder-Mead algorithm for unconstrained derivative-free optimization. In the description of the algorithm, the word *continue* will be used to mean that we move to the next iteration. (It corresponds to the MATLAB command of the same name.) The input of the algorithm is:

- a function f of n variables,
- n+1 points $x_i \in \mathbb{R}^n$ such that the directions $x_j x_1$ are linearly independent (we will store them in an $(n+1) \times n$ matrix
- four design parameters,

$$\mu_{\text{ref}} = 1, \quad \mu_{\text{exp}} = 2, \quad \mu_{\text{con}} = \frac{1}{2}, \quad \mu_{\text{int}} = -\frac{1}{2}$$

- a tolerance value
- a value for the maximum number of evaluations of f.

We will also need a sorting routine: given the n + 1 points x_i and the values $v_i = f(x_i)$, by sorting we mean to reorder the points so that

$$v_1 \le v_2 \le \ldots \le v_{n+1}.$$

This can be easily done using the MATLAB function **sort**. Some expressions will be shortened for better visibility of the algorithm.

compute $v_i = f(x_i)$ for $i = 1, \ldots, n+1$ while $v_{\max} - v_{\min} > \text{tol}$ sort the points $\overline{x} = \frac{1}{n} \sum_{j=1}^{n} x_j$ $d = \overline{x} - x_{n+1}$ $x_{\rm ref} = \overline{x} + \mu_{\rm ref} d$ $v_{\rm ref} = f(x_{\rm ref})$ if $v_1 \leq v_{\text{ref}} < v_n$ $(x_{n+1}, v_{n+1}) = (x_{ref}, v_{ref})$ % reflection continue % expension else if $v_{\rm ref} < v_1$ $x_{\exp} = \overline{x} + \mu_{\exp} d$ $v_{\rm exp} = f(x_{\rm ref})$ $(x_{n+1}, v_{n+1}) = \text{best of } (x_{\exp}, v_{\exp}) \text{ and } (x_{\mathrm{ref}}, v_{\mathrm{ref}})$ continue else if $v_n \leq v_{ref} < v_{n+1}$ % contraction $x_{\rm con} = \overline{x} + \mu_{\rm con} d$ $v_{\rm con} = f(x_{\rm con})$ if $v_{\rm con} < v_{\rm ref}$ $(x_{n+1}, v_{n+1}) = (x_{\text{con}}, v_{\text{con}})$ continue end else if $v_{\text{ref}} > v_{n+1}$ % interior contraction $x_{\text{int}} = \overline{x} + \mu_{\text{int}} d$ $v_{\text{int}} = f(x_{\text{int}})$ if $v_{\text{int}} < v_{n+1}$ $(x_{n+1}, v_{n+1}) = (x_{\text{int}}, v_{\text{int}})$ continue end end compute $x_i = x_1 + \frac{1}{2}(x_i - x_1)$ for i = 2, ..., n + 1% shrinking compute $v_i = f(x_i)$ for $i = 2, \ldots, n+1$ end

The algorithm should also be complemented with a counter of the number of evaluations of f. Once this value is larger that the limit we had input, the code should stop.