The Nelder-Mead Simplex Method

$1 \quad 2 \quad 1/2 \quad 1/2$ ← typical values

① Choose $0 < \alpha < \gamma$, $0 < \beta < 1$, $0 < \delta < 1$.

Given simplex $Y = \{x_0, x_1, x_2, \cdots, x_n\} \subseteq \mathbb{R}^n$

② Determine x_B satisfying $f(x_B) \leq f(x_k)$ for all $x_k \in Y$ (BEST)

x_W satisfying $f(x_W) \geq f(x_k)$ for all $x_k \in Y$ (WORST)

x_S satisfying $f(x_S) \geq f(x_k)$ for all $x_k \in Y$, $x_k \neq x_W$ (second worst)

$$x_C = \frac{1}{n} \sum_{\substack{k=0 \\ \neq W}}^{n} x_k$$ (CENTROID OF ALL BUT WORST)

③ (REFLECT) $x_R = x_C + \alpha(x_C - x_W)$.

④ If $f(x_B) \leq f(x_R) < f(x_S)$ then $Y = (Y \setminus \{x_W\}) \cup \{x_R\}$, goto step 2.

⑤ If $f(x_R) < f(x_B)$ then (EXPAND) $x_E = x_C + \gamma(x_C - x_W)$.

⑥ If $f(x_E) < f(x_R)$ then $Y = (Y \setminus \{x_W\}) \cup \{x_E\}$, goto step 2,

else $Y = (Y \setminus \{x_W\}) \cup \{x_R\}$, goto step 2.

⑦ If $f(x_S) \leq f(x_R) < f(w)$ then (OUTSIDE CONTRACT) $x_{OC} = x_C + \beta(x_R - x_C)$.

⑧ If $f(x_{OC}) \leq f(x_R)$ then $Y = (Y \setminus \{x_W\}) \cup \{x_{OC}\}$, goto step 2.

⑨ (INSIDE CONTRACT) $x_{IC} = x_C + \beta(x_W - x_C)$.

⑩ If $f(x_{IC}) < f(x_W)$ then $Y = (Y \setminus \{x_W\}) \cup \{x_{IC}\}$, goto step 2.

⑪ (SHRINK) $x_k \leftarrow x_k + \delta(x_B - x_k)$ for all $x_k \in Y$, goto step 2.

Notes:

- All except step ⑪ can be accomplished with little computational effort.
- Shrink steps appear to be rare in practice.
- Convergence results are very limited and weak.
- McKinnon (1998) example – strictly convex twice continuously differentiable function on which N-M fails to converge to the minimizer.
- Use N-M as a fast alternative to find a warm start to a gradient-based method.
- High computational overhead to get started.