Notes on NEWUOA

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How to terminate? Is $\|\nabla Q_k(x_k)\| \leq \eta\Delta_k$ attainable? What about $\|\nabla Q_k(x_k)\| \leq \epsilon$? What about $\|x_k^+ - x_k\| \leq \eta\Delta_k$?

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Algorithm 0.1

?⟨alg:newuoa⟩? Input $\Delta_0 \in (0, +\infty)$, $m \in \{n+2, n+3, \ldots, (n+1)(n+2)/2\}$, and $\mathcal{X}_0 \subset \mathbb{R}^n$ with $x_0 \in \mathcal{X}_0$ and $|\mathcal{X}_0| = m$. Set $Q_{-1} = 0$ and $k = 0$.

1. Pick $Q_k \in \{Q \in \mathcal{Q} : Q(x) = f(x) \text{ for all } x \in \mathcal{X}_k\}$. Define $x_k = \operatorname{argmin}\{f(x) : x \in \mathcal{X}_k\}$.
2. If $\tau_k = 1$, then

$$x_k^+ \approx \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \le \Delta_k\}, \tag{0.1}$$?eq:?

$$x_k^- \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k, x_k^+, x) : x \in \mathcal{X}_k\}, \tag{0.2}$$?eq:?

$$\rho_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]. \tag{0.3}$$?eq:?

   If $\|x_k^+ - x_k\| \le \alpha\Delta_k$, then set $\tau_{k+1} = 0$, $\mathcal{X}_{k+1} = \mathcal{X}_k$; otherwise, set

$$\mathcal{X}_{k+1} = \begin{cases} \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\} & \text{if } \rho_k > 0 \text{ or } \kappa(\mathcal{X}_k, x_k^+, x_k^-) < \kappa_0, \\ \mathcal{X}_k, & \text{else.} \end{cases} \tag{0.4}$$?eq:?

   Increment k. Go to Step 1.
3. If $\tau_k = 0$, then

$$x_k^- = \operatorname{argmax}\{\|x - x_k\| : x \in \mathcal{X}_k\}, \tag{0.5}$$?eq:?

$$x_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k, x, x_k^-) : \|x - x_k\| \le \Delta_k\} \tag{0.6}$$?eq:?

$$\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\} \tag{0.7}$$?eq:?

$$\tau_{k+1} = 1. \tag{0.8}$$?eq:?

4. If $\|x_k^+ - x_k\| \ge \alpha\Delta_k$, then

$$x_k^- \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k, x_k^+, x) : x \in \mathcal{X}_k\}. \tag{0.9}$$?eq:?

   If $\kappa(\mathcal{X}_k, x_k^+, x_k^-) \le \kappa_0$ or $f(x_k^+) < f(x_k)$, then $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}$.
5. If $\|x_k^+ - x_k\| < \eta\Delta_k$ or $\rho_k \le 0$ and $\kappa_k \ge \kappa_0$, then set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}$. Otherwise, set $y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \mathcal{X}_k\}$, $y_k^+ = \operatorname{argmin}\{\kappa(\mathcal{X}_k, y, y_k^-) : \|y - x_k\| \le \Delta_k\}$, and $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{y_k^+\} \setminus \{y_k^-\}$. Increment k. Go to Step 1.