Notes on NEWUOA

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Algorithm 0.1

?⟨alg:newuoa⟩? Input $\Delta_0 \in (0, +\infty)$, $m \in \{n+2, n+3, \dots, (n+1)(n+2)/2\}$, 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:?

Set

$$\tau_{k+1} = [\|x_k^+ - x_k\| > \alpha\Delta_k] \wedge [\rho_k > 0 \vee \kappa(\mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}) < \kappa_0] \tag{0.4}$$?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

$$\mathcal{X}_{k+1} = \begin{cases} \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\} & \text{if } \rho_k > 0 \text{ or } \kappa(\mathcal{X}_k, x_k^+, x_k^-) < \kappa_0, \\ \mathcal{X}_k, & \text{else.} \end{cases} \tag{0.5}$$?eq:?

3. If $\tau_k = 0$, then

$$x_k^- = \operatorname{argmax}\{\|x - x_k\| : x \in \mathcal{X}_k\}, \tag{0.6}$$?eq:?

$$x_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k, x, x_k^-) : \|x - x_k\| \le \Delta_k\} \tag{0.7}$$?eq:?

and set

$$\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}, \Delta_{k+1} = \Delta_k, \tau_{k+1} = 1. \tag{0.8}$$?eq:?

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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 $\|x_k^+ - x_k\| \leq \eta\Delta_k$?