Notes on NEWUOA

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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 $|\mathcal{X}_0| = m$. Set $Q_{-1} = 0$ and $k = 0$.

1. **Model construction**. Pick $Q_k \in \{Q \in \mathcal{Q} : Q(x) = f(x) \text{ for all } x \in \mathcal{X}_k\}$.
2. **Trust-region step**. Define $x_k = \operatorname{argmin}\{f(x) : x \in \mathcal{X}_k\}$. Calculate

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

   If $\|x_k^+ - x_k\| \le \alpha\Delta_k$, then set $\Delta_{k+1} = \theta\Delta_k$, and exit if $\Delta_{k+1} \le \tau$. Otherwise, update Δ_k to Δ_{k+1} according to $\rho_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$.
3. **Interpolation set update.** If $\|x_k^+ - x_k\| \ge \alpha\Delta_k$, then calculate

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

   and set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}$ if $\rho_k > 0$ or $\kappa(\mathcal{X}_k, x_k^+, x_k^-) < \kappa_0$.
4. **Geometry improvement**. If $\|x_k^+ - x_k\| \le \alpha\Delta_k$, or $\|x_k^+ - x_k\| > \alpha\Delta_k$ but $\rho_k \le 0$ and $\kappa(\mathcal{X}_k, x_k^+, x_k^-) \ge \kappa_0$, then calculate

$$y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \mathcal{X}_k\}, \tag{0.3}$$?eq:?

$$y_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k, y, y_k^-) : \|y - x_k\| \le \Delta_k\}, \tag{0.4}$$?eq:?

   and set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{y_k^+\} \setminus \{y_k^-\}$.

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

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