Notes on NEWUOA

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Algorithm 0.1 OPTimization based on Interpolation Models (OPTIM)

?⟨alg:optim⟩? Input $\Delta_0 \in (0, +\infty)$, $\tau > 0$, $m \in \{n+2, n+3, \ldots, (n+1)(n+2)/2\}$, and $\mathcal{X}_0 \subset \mathbb{R}^n$ with $|\mathcal{X}_0| = m$ and $\kappa(\mathcal{X}_0) \le \kappa_0$. 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 evaluation**. 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:xget?

   If $\|x_k^+ - x_k\| < \alpha\Delta_k$, then set $\Delta_{k+1} = \theta\Delta_k$. 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

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

?eq:xdrop?

   and set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup x_k^+ \setminus x_k^-$ if $\rho_k > 0$ or $\kappa(\mathcal{X}_k \cup x_k^+ \setminus x_k^-) \le \kappa_0$.

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

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

?eq:ydrop?

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

?eq:yget?

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

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Algorithm 0.2 NEWUOA

?⟨alg:newuoa⟩? Input $\Delta_0 \in (0, +\infty)$, $\tau > 0$, $m \in \{n+2, n+3, \dots, (n+1)(n+2)/2\}$, and $\mathcal{X}_0 \subset \mathbb{R}^n$ with $|\mathcal{X}_0| = m$ and $\kappa(\mathcal{X}_0) \le \kappa_0$. 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 evaluation**. Define $x_k = \operatorname{argmin}\{f(x) : x \in \mathcal{X}_k\}$. Calculate

$$x_k^+ \approx \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \le \Delta_k\}. \tag{0.5}$$?eq:xgetn?

   If $\|x_k^+ - x_k\| < \alpha\Delta_k$, then set $\Delta_{k+1} = \theta\Delta_k$. 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

$$x_k^- \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup x_k^+ \setminus x) : x \in \mathcal{X}_k\}, \tag{0.6}$$?eq:xdropn?

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

$$y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \mathcal{X}_k\}, \tag{0.7}$$?eq:ydropn?

$$y_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup y \setminus y_k^-) : \|y - x_k\| \le \Delta_k\}, \tag{0.8}$$?eq:ygetn?

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