

Notes on NEWUOA

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Algorithm 0.1 OPTimization based on Interpolation Models (OPTIM)

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

$$x_k^+ \approx \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \leq \Delta_k\}. \quad (0.1) \text{ ?eq:xget?}$$

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 $r_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$.

3. **Interpolation set update.** If $\|x_k^+ - x_k\| \geq \alpha\Delta_k$, then calculate

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

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

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

$$y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \mathcal{X}_k\}, \quad (0.3) \text{ ?eq:ydrop?}$$

$$y_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup y \setminus y_k^-) : \|y - x_k\| \leq \Delta_k\}, \quad (0.4) \text{ ?eq:yget?}$$

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

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Algorithm 0.2 NEWUOA

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 $\kappa(\mathcal{X}_0) \leq \kappa_0$. 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

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

If $\|x_k^+ - x_k\| < \rho_k/2$, then set $\mathbf{s}_k = 1$; otherwise, set $\mathbf{s}_k = 0$. If $\mathbf{s}_k = 1$ and the errors in recent models are sufficiently small, then set $\mathbf{r}_k = 1$; otherwise, set $\mathbf{r}_k = 0$. If $\mathbf{s}_k = 1$ and $\mathbf{r}_k = 0$, then set $\Delta_{k+1} = \max\{\Delta_k/10, \rho_k\}$. If $\mathbf{s}_k = 0$, then calculate $r_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$.

3. **Interpolation set update.** If $\|x_k^+ - x_k\| \geq \alpha\Delta_k$, then calculate

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

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

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

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

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

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