

Notes on NEWUOA

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We define $\bar{\mathcal{X}}_k$ to be a point in \mathcal{X}_k such that

$$f(\bar{\mathcal{X}}_k) = \min\{f(x) : x \in \mathcal{X}_k\}. \quad (0.1) \text{?eq:xopt?}$$

If multiple points attain the minimum, then we take the earliest one visited by the algorithm.

$$\delta(\mathcal{X}_k) = \max\{\|x - \bar{\mathcal{X}}_k\| : x \in \mathcal{X}_k\} \quad (0.2) \text{?eq:xdist?}$$

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Algorithm 0.1 OPTimization based on Interpolation Models (OPTIM)

$\langle \text{alg:optim} \rangle?$ 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 $k = 0$.

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

$$x_k^g \approx \operatorname{argmin}\{Q_k(x) : \|x - \bar{\mathcal{X}}_k\| \leq \Delta_k\}. \quad (0.3) \text{ ?eq:xget?}$$

If $\|x_k^g - \bar{\mathcal{X}}_k\| < \alpha\Delta_k$, then set $\Delta_{k+1} = \theta\Delta_k$. Otherwise, update Δ_k to Δ_{k+1} according to $r_k = [f(\bar{\mathcal{X}}_k) - f(x_k^g)]/[Q_k(\bar{\mathcal{X}}_k) - Q_k(x_k^g)]$.

3. **Interpolation set update.** If $\|x_k^g - \bar{\mathcal{X}}_k\| \geq \alpha\Delta_k$, then calculate

$$x_k^d \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup x_k^g \setminus x) : x \in \mathcal{X}_k\}, \quad (0.4) \text{ ?eq:xdrop?}$$

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

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

$$y_k^d = \operatorname{argmax}\{\|y - \bar{\mathcal{X}}_k\| : y \in \mathcal{X}_k\}, \quad (0.5) \text{ ?eq:ydrop?}$$

$$y_k^g \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup y \setminus y_k^d) : \|y - \bar{\mathcal{X}}_k\| \leq \Delta_k\}, \quad (0.6) \text{ ?eq:yget?}$$

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

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 $\kappa(\mathcal{X}_0) \leq \kappa_0$. Define $Q_0 = \operatorname{argmin}\{\|\nabla^2 Q\|_F : Q \in \mathcal{Q} \text{ and } Q(x) = f(x) \text{ for } x \in \mathcal{X}_0\}$. Set $k = 0$.

1. **Trust-region step evaluation.** Set

$$x_k^g \approx \operatorname{argmin}\{Q_k(x) : \|x - \bar{\mathcal{X}}_k\| \leq \Delta_k\}. \quad (0.7) \text{?eq:xgetn?}$$

$$S = \mathbb{1}(\|x_k^g - \bar{\mathcal{X}}_k\| < \rho_k/2), \quad (0.8) \text{?eq:shortd?}$$

$$R = \mathbb{1}(S = 1 \text{ and the errors in recent models are small}). \quad (0.9) \text{?eq:redrho?}$$

If $R = 1$, then set $\mathcal{X}_{k+1} = \mathcal{X}_k$, $Q_{k+1} = Q_k$, and go to step 4. If $S = 1$ and $R = 0$, then set $\Delta_{k+1} = \max\{\Delta_k/10, \rho_k\}$. If $S = 0$, then evaluate $r_k = [f(\bar{\mathcal{X}}_k) - f(x_k^g)]/[Q_k(\bar{\mathcal{X}}_k) - Q_k(x_k^g)]$ and update Δ_k to Δ_{k+1} according to r_k .

2. **Interpolation set and model update.** If $S = 0$, then calculate

$$x_k^d \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup x_k^g \setminus x) : x \in \mathcal{X}_k\}, \quad (0.10) \text{?eq:xdropt?}$$

and let $\mathcal{X}_k^+ = \mathcal{X}_k \cup x_k^g \setminus x_k^d$ if $r_k > 0$ or $\kappa(\mathcal{X}_k \cup x_k^g \setminus x_k^d) \leq \kappa_0$. In any other case, $\mathcal{X}_k^+ = \mathcal{X}_k$. Set

$$Q_k^+ = \operatorname{argmin}\{\|\nabla^2 Q - \nabla^2 Q_k\|_F : Q \in \mathcal{Q} \text{ and } Q(x) = f(x) \text{ for } x \in \mathcal{X}_k^+\}. \quad (0.11) \text{?eq:updateeq1?}$$

3. **Geometry improvement.** If $\delta(\mathcal{X}_k^+) \geq 2\Delta_{k+1}$ and either $S = 1$ or $r_k < 1/10$, then calculate

$$y_k^d = \operatorname{argmax}\{\|y - \bar{\mathcal{X}}_k^+\| : y \in \mathcal{X}_k^+\}, \quad (0.12) \text{?eq:ydropt?}$$

$$y_k^g \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k^+ \cup y \setminus y_k^d) : \|y - \bar{\mathcal{X}}_k^+\| \leq \Delta_k^+\} \quad (0.13) \text{?eq:ygetn?}$$

with $\Delta_k^+ = \max\{\min\{\delta(\mathcal{X}_k^+)/10, \Delta_{k+1}/2\}, \rho_k\}$, and set

$$\mathcal{X}_{k+1} = \mathcal{X}_k^+ \cup y_k^g \setminus y_k^d, \quad (0.14) \{?\}$$

$$Q_{k+1} = \operatorname{argmin}\{\|\nabla^2 Q - \nabla^2 Q_k^+\|_F : Q = f \text{ on } \mathcal{X}_{k+1}, Q \in \mathcal{Q}\}. \quad (0.15) \{?\}$$

Otherwise, $\mathcal{X}_{k+1} = \mathcal{X}_k^+$ and $Q_{k+1} = Q_k^+$. If $\delta(\mathcal{X}_k^+) < 2\Delta_{k+1}$ and either $S = 1$ or $r_k \leq 0$, then set R to 1.

4. **Resolution enhancement.** If $R = 1$, then reduce ρ_k by about a factor of 10 to obtain ρ_{k+1} , and set $\Delta_{k+1} = \max\{\rho_{k+1}/2, \rho_k\}$. If $R = 0$, then set $\rho_{k+1} = \rho_k$.
