

# Notes on NEWUOA

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**Algorithm 0.1** OPTimization based on Interpolation Models (OPTIM)

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?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  $\Delta_k$  to  $\Delta_{k+1}$  according to  $\rho_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$ .

3. **Interpolation set update.** If  $\|x_k^+ - x_k\| \geq \alpha\Delta_k$ , 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  $\rho_k > 0$  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

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

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

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

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**Algorithm 0.2** NEWUOA

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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

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

Let  $s_k = \mathbb{1}(\|x_k^+ - x_k\| < \rho_k/2)$ , then set  $\Delta_{k+1} = \theta \Delta_k$ . Otherwise, update  $\Delta_k$  to  $\Delta_{k+1}$  according to  $\rho_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$ .

3. **Interpolation set update.** If  $\|x_k^+ - x_k\| \geq \alpha \Delta_k$ , 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  $\mathcal{X}_{k+1} = \mathcal{X}_k \cup y_k^+ \setminus y_k^-$ .

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