

# Notes on NEWUOA

Zaikun Zhang \*

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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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\*Hong Kong Polytechnic University, [zaikun.zhang@polyu.edu.hk](mailto:zaikun.zhang@polyu.edu.hk)

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

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$\langle \text{alg:optim} \rangle?$  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  $\Delta_k$  to  $\Delta_{k+1}$  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  $\mathcal{X}_{k+1} = \mathcal{X}_k \cup y_k^g \setminus y_k^d$ .

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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  $\kappa(\mathcal{X}_0) \leq \kappa_0$ . 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  $R = 0$  and  $S = 1$ , 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  $\Delta_k$  to  $\Delta_{k+1}$  according to  $r_k$ .

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

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

If  $S = 0$  and either  $r_k > 0$  or  $\kappa(\mathcal{X}_k \cup x_k^g \setminus x_k^d) \leq \kappa_0$ , then set

$$\mathcal{X}_k^+ = \mathcal{X}_k \cup x_k^g \setminus x_k^d, \quad Q_k^+ = \operatorname{argmin}\left\{\|Q - Q_k\|_S : Q|_{\mathcal{X}_k^+} = f|_{\mathcal{X}_k^+}, Q \in \mathcal{Q}\right\}; \quad (0.11) \text{?eq:updateeq1?}$$

otherwise,  $\mathcal{X}_k^+ = \mathcal{X}_k$  and  $Q_k^+ = Q_k$ .

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

$$\mathcal{X}_{k+1} = \mathcal{X}_k^+ \cup y_k^g \setminus y_k^d, \quad Q_{k+1} = P_{\mathcal{Q}_{k+1}}^S(Q_k^+); \quad (0.14) \text{?eq:??}$$

otherwise,  $\mathcal{X}_{k+1} = \mathcal{X}_k^+$  and  $Q_{k+1} = Q_k^+$ . If  $\delta(\mathcal{X}_k^+) < 2\Delta_{k+1}$ ,  $\max\{\Delta_{k+1}, \|x_k^g - \bar{\mathcal{X}}_k\|\} \leq \rho_k$ , and either  $S = 1$  or  $r_k \leq 0$ , then set  $R$  to 1.

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

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