Notes on NEWUOA

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June 8, 2021 1:34pm

Algorithm 0.1

?⟨alg:newuoa⟩? Input $\Delta_0 \in (0, +\infty)$, $m \in \{n+2, n+3, \ldots, (n+1)(n+2)/2\}$, and $\mathcal{X}_0 \subset \mathbb{R}^n$ with $x_0 \in \mathcal{X}_0$ and $|\mathcal{X}_0| = m$. Set $Q_{-1} = 0$ and $k = 0$.

1. $x_k = \operatorname{argmin}\{f(x) : x \in \mathcal{X}_k\}$
2. $Q_k = \operatorname{argmin}\{\|\nabla^2 Q - \nabla^2 Q_{k-1}\|_{\mathrm{F}} : Q \in \mathcal{Q} \text{ and } Q(x) = f(x) \text{ for } x \in \mathcal{X}_k\}$.
3. $x_k^+ = \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \le \Delta_k\}$, $x_k^- = \operatorname{argmin}\{\kappa(\mathcal{X}_k, x_k^+, x) : x \in \mathcal{X}_k \setminus \{x_k\}\}$,
4. If $\|x_k^+ - x_k\| \ge \eta\Delta_k$ then $\kappa_k = \kappa(\mathcal{X}_k, x_k^+, x_k^-)$, $\rho_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$, else $\kappa_k = +\infty$, $\rho_k = -\infty$.
5. If $\rho_k > 0$ or $\kappa_k < \kappa_0$, then set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{x_k^+\} \setminus \{x_k^-\}$. Otherwise, set $y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \mathcal{X}_k\}$, $y_k^+ = \operatorname{argmin}\{\kappa(\mathcal{X}_k, y, y_k^-) : \|y - x_k\| \le \Delta_k\}$, and $\mathcal{X}_{k+1} = \mathcal{X}_k \cup \{y_k^+\} \setminus \{y_k^-\}$. Increment k. Go to Step 1.

How to terminate? Is $\|\nabla Q_k(x_k)\| \le \eta\Delta_k$ attainable? What about $\|\nabla Q_k(x_k)\| \le \epsilon$? What about $\|x_k^+ - x_k\| \le \eta\Delta_k$?

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