Notes on NEWUOA

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June 12, 2021 5:04pm

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 $\kappa(\mathcal{X}_0) \le \kappa_0$. Set $k = 0$.

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

$$x_k^+ \approx \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \le \Delta_k\}. \tag{0.1}$$?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 $\|x_k^+ - x_k\| \ge \alpha\Delta_k$, then calculate

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

   and set $\mathcal{X}_{k+1} = \mathcal{X}_k \cup x_k^+ \setminus x_k^-$ if $r_k > 0$ or $\kappa(\mathcal{X}_k \cup x_k^+ \setminus x_k^-) \le \kappa_0$.
4. **Geometry improvement**. If $\|x_k^+ - x_k\| < \alpha\Delta_k$, or $\|x_k^+ - x_k\| > \alpha\Delta_k$ but $r_k \le 0$ and $\kappa(\mathcal{X}_k \cup x_k^+ \setminus x_k^-) > \kappa_0$, then calculate

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

$$y_k^+ \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup y \setminus y_k^-) : \|y - x_k\| \le \Delta_k\}, \tag{0.4}$$?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

?⟨alg:newuoa⟩? Input $\Delta_0 \in (0, +\infty)$, $\tau > 0$, $m \in \{n+2, n+3, \ldots, (n+1)(n+2)/2\}$, and $\mathcal{X}_0 \subset \mathbb{R}^n$ with $|\mathcal{X}_0| = m$ and $\kappa(\mathcal{X}_0) \leq \kappa_0$. Define $Q_0 = \operatorname{argmin}\{\|\nabla Q\|_{\mathrm{F}} : Q \in \mathcal{Q} \text{ and } Q(x) = f(x) \text{ for all } x \in \mathcal{X}_0\}$. Set $k = 0$.

1. **Trust-region step evaluation**. Define $x_k = \operatorname{argmin}\{f(x) : x \in \mathcal{X}_k\}$. Calculate
$$x_k^+ \approx \operatorname{argmin}\{Q_k(x) : \|x - x_k\| \leq \Delta_k\}. \tag{0.5}$$
?eq:xgetn?
Set $\mathsf{S}_k = \mathbb{1}(\|x_k^+ - x_k\| < \rho_k/2)$, $\mathtt{R}_k = \mathbb{1}(\mathsf{S}_k = 1 \text{ and the errors in recent models are small})$. If $\mathsf{S}_k = 1$ and $\mathtt{R}_k = 0$, then set $\Delta_{k+1} = \max\{\Delta_k/10, \rho_k\}$. If $\mathsf{S}_k = 0$, then evaluate $r_k = [f(x_k) - f(x_k^+)]/[Q_k(x_k) - Q_k(x_k^+)]$, and update Δ_k to Δ_{k+1} according to r_k.
2. **Interpolation set update**. If $\mathsf{S}_k = 0$, then calculate
$$x_k^- \approx \operatorname{argmin}\{\kappa(\mathcal{X}_k \cup x_k^+ \setminus x) : x \in \mathcal{X}_k\}, \tag{0.6}$$
?eq:xdropn?
and take $\hat{\mathcal{X}}_k = \mathcal{X}_k \cup x_k^+ \setminus x_k^-$ if $r_k > 0$ or $\kappa(\mathcal{X}_k \cup x_k^+ \setminus x_k^-) \leq \kappa_0$. In any other case, $\hat{\mathcal{X}}_k = \mathcal{X}_k$. Set
$$\hat{Q}_k = \operatorname{argmin}\{\|Q - Q_k\|_{\mathrm{F}} : Q \in \mathcal{Q} \text{ and } Q(x) = f(x) \text{ for all } x \in \hat{\mathcal{X}}_k\}. \tag{0.7}$$
?eq:updateq1?
3. **Geometry improvement**. If $\mathtt{R}_k = 0$ and either $\mathsf{S}_k = 1$ or $r_k < 1/10$, then set
$$y_k^- = \operatorname{argmax}\{\|y - x_k\| : y \in \hat{\mathcal{X}}_k\}. \tag{0.8}$$
?eq:ydropn?
If $\|y_k^- - x_k\| \geq 2\Delta_{k+1}$, then define $\bar{\Delta}_k = \max\{\rho_k, \min\{\|y_k^- - x_k\|/10, \Delta_{k+1}/2\}\}$, calculate
$$y_k^+ \approx \operatorname{argmin}\{\kappa(\hat{\mathcal{X}}_k \cup y \setminus y_k^-) : \|y - x_k\| \leq \bar{\Delta}_k\}, \tag{0.9}$$
?eq:ygetn?
and set $\mathcal{X}_{k+1} = \hat{\mathcal{X}}_k \cup y_k^+ \setminus y_k^-$.
4. **Resolution enhancement**. If $\mathtt{R}_k = 1$, 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 $\mathtt{R}_k = 0$, then set $\rho_{k+1} = \rho_k$.