数理解析研究所講究録
第2011巻 2016年 47-56

On global minimization for general $p-$regularized subproblems with $p > 2$

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Abstract

The p-regularized subproblem (p-RS) is a regularizing term for computing a Newton-like step for unconstrained optimization, which incorporates a weighted regularization term $\frac{\sigma}{p}\|x\|^p$. In this article, we resolve the global minimizers of (p-RS) for $p > 2$ with necessary and sufficient optimality conditions.

Key Words: Trust-region subproblem; Local minimizer; Extended Trust-region subproblem.

1 Introduction

For an unconstrained optimization problem to minimize f over $\mathbb{R}^n$, Newton's method has an attractive local convergence property near a second order critical point. Ensuring the global convergence for Newton's method with an analyzable computational complexity, however, requires modifications to guarantee a *sufficient* descent at each step. Unlike the Levenberg-Marquardt type of methods or most quasi-Newton methods which always maintain a positive-definite approximate Hessian of f, the p-regularized subproblem minimizes globally the second order Taylor's polynomial of f plus a weighted (by σ) higher order regularization term. The subproblem takes the following model

$$\text{(p−RS)} \quad \min_{x\in\mathbb{R}^n} \left\{ g(x) = \frac{1}{2}x^T Hx + c^T x + \frac{\sigma}{p}\|x\|^p \right\},$$

where $\sigma > 0$, $p > 2$, and H is the Hessian of f at any iterate, regardless of its definiteness. It is often assumed that f is smooth enough to have a symmetric Hessian and to obtain the desired global convergence. If the global minimizer of (p-RS) renders a satisfactory decrease in the value of f, it is accepted; but rejected otherwise with an increase in σ to enhance the regularization force.

In literature, (p-RS) with $p = 3$ is known as the cubic regularization which is the most common choice among all others. The idea of the cubic regularization was first due to Griewank [9] and later was considered by many authors with thorough global convergence and complexity analysis. See Nesterov and Polyak [15]; Weiser Deuflhard and Erdmann [17]; and Cartis, Gould and Toint [2]. When $p = 4$, (p-RS) reduces to a form of the double well potential function which has many applications in solid mechanics and quantum mechanics [5, 18]. Gould, Robinson and Thorne [8] studied (p-RS) for a general $p > 2$ in comparison with the the trust-region subproblem

$$\begin{array}{lll} \text{(TRS)} & \min & \frac{1}{2}x^T Hx + c^T x \\ & \text{s. t.} & \|x\|^2 \le \Delta, \ x \in \mathbb{R}^n. \end{array}$$

In this article, we characterize (p-RS) completely for any $p > 2$ by (i) extending the necessary and sufficient global optimality conditions for $p = 3$ in [2] and (ii) the analysis using the secular function (to be specified later) for $p = 4$ in [18].

Notations. Let $v(\cdot)$ denote the optimal value of problem $(\cdot)$. For any symmetric matrix $P \in \mathbb{R}^{n\times n}$, $P \succ (\succeq) 0$ means that P is positive (semi)definite. The determinant of P is denoted by $\det(P)$ whereas the identity matrix of order n by I. For a vector $x \in \mathbb{R}^n$, $\mathrm{Diag}(x)$ is a diagonal matrix with diagonal components being $x_1, \ldots, x_n$. For a number $\beta \in \mathbb{R}$, $\mathrm{sign}(\beta) = \frac{\beta}{|\beta|}$ if $\beta \neq 0$, otherwise $\mathrm{sign}(\beta) = 0$. Finally, $\lambda_i(P)$ is the ith smallest eigenvalue of P.

2 Main results for global minimization

We first observe that the objective function $g(x)$ of (p-RS) is coercive, i.e.,

$$\lim_{\|x\|\to+\infty} g(x) = +\infty.$$

Consequently, the global minimizer of (p-RS) always exists. The starting point of the analysis is the first order and the second order necessary conditions for any local minimizer of g.

Lemma 1 *Assume that $\underline{x}$ is a local minimizer of (p-RS), $p > 2$. It holds that*

$$\nabla g(\underline{x}) = \left(H + \sigma\|\underline{x}\|^{p-2}I\right)\underline{x} + c = 0, \tag{1}$$

$$\nabla^2 g(\underline{x}) = (H + \sigma\|\underline{x}\|^{p-2}I) + \sigma(p-2)\|\underline{x}\|^{p-4}\underline{x}\underline{x}^T \succeq 0, \tag{2}$$

where ∇g, $\nabla^2 g$ denote the gradient and the Hessian of $g(x)$, respectively.

The next theorem shows that, a local minimizer $\underline{x}$ becomes global if and only if $H + \sigma\|\underline{x}\|^{p-2}I \succeq 0$. The necessity has been shown by Theorem 2 in [8]. We only prove the sufficiency here.

Theorem 1 *The point x^* is a global minimizer of (p-RS) for $p > 2$ if and only if it is a critical point satisfying $\nabla g(x^*) = 0$ and $H + \sigma\|x^*\|^{p-2}I \succeq 0$. Moreover, the ℓ_2 norms of all the global minimizers are equal.*

Proof If $x^* = 0_n$, then $\sigma\|x^*\|^{p-2} = 0$ so that $c = -(H + \sigma\|x^*\|^{p-2}I)x^* = 0$ and $H = H + \sigma\|x^*\|^{p-2}I \succeq 0$. Consequently, $x^THx \geq 0$, $\forall x \in \mathbb{R}^n$. It follows that $x^* = 0_n$ is a global minimizer since

$$g(x) = \frac{1}{2}x^THx + c^Tx + \frac{\sigma}{p}\|x\|^p \geq \frac{\sigma}{p}\|x\|^p > 0 = g(0), \ \forall x \neq 0_n = x^*.$$

Now we assume $x^* \neq 0_n$, i.e., $\|x^*\| > 0$. Define $Q = H + \sigma\|x^*\|^{p-2}I$. According to the assumption, $Q \succeq 0$. Then, for any $x \in \mathbb{R}^n$ and $x \neq x^*$, it holds that

$$\begin{aligned} g(x) &= \frac{1}{2}x^T Hx + c^T x + \frac{\sigma}{p}\|x\|^p \\ &= \frac{1}{2}x^T Qx + c^T x - \frac{1}{2}(\sigma\|x^*\|^{p-2})x^T x + \frac{\sigma}{p}\|x\|^p \\ &= \frac{1}{2}x^T Qx + c^T x + \frac{\sigma}{p}\|x^*\|^p \left(\left(\frac{\|x\|^2}{\|x^*\|^2} \right)^{\frac{p}{2}} - \frac{p}{2}\frac{\|x\|^2}{\|x^*\|^2} \right) \end{aligned} \tag{3}$$

Define $f(t) = t^{\frac{p}{2}}$, $p > 2$. It is strictly convex for $t > 0$. Therefore,

$$f(t) = t^{\frac{p}{2}} \geq f(1) + f'(1)(t-1) = 1 + \frac{p}{2}(t-1), \ \forall t > 0.$$

By substituting t with $\frac{\|x\|^2}{\|x^*\|^2}$, we have

$$\left(\frac{\|x\|^2}{\|x^*\|^2} \right)^{\frac{p}{2}} - \frac{p}{2}\frac{\|x\|^2}{\|x^*\|^2} \geq 1 - \frac{p}{2}.$$

Then,

$$g(x) \geq \frac{1}{2}x^T Qx + c^T x + \frac{\sigma}{p}\|x^*\|^p(1 - \frac{p}{2}). \tag{4}$$

By $Q \succeq 0$, the lower bounding function of g in the right hand side of (4) is convex quadratic in terms of x. Since x^* satisfies $(H + \sigma\|x^*\|^{p-2}I)x^* = Qx^* = -c$, x^* is a global minimizer of the convex function in the right hand side of (4). As a consequence,

$$g(x) \geq \frac{1}{2}(x^*)^T Qx^* + c^T x^* + \frac{\sigma}{p}\|x^*\|^p(1 - \frac{p}{2}) = g(x^*)$$

and x^* is a global minimizer of (p-RS).

Finally, from (3), if $\hat{x}$ is also a global minimizer of (p-RS), $\hat{x}$ must minimize both $\frac{1}{2}x^T Qx + c^T x$ and $\left(\frac{\|x\|^2}{\|x^*\|^2}\right)^{\frac{p}{2}} - \frac{p}{2}\frac{\|x\|^2}{\|x^*\|^2}$ simultaneously. This can happen if and only if $Q\hat{x} = -c$ and $\|\hat{x}\| = \|x^*\|$.

Remark 1 *When $p = 3$, two other proofs of the necessary and sufficient condition can be found in Theorem 3.1 in [2] and Theorem 10 in [15], respectively. We notice that the proof* *in [2] is inherited from that of the necessary and sufficient condition for the trust-region subproblem [3] and the proof in [15] highly relies on the special structure of the case $p = 3$. Our proof is much easier in understanding, since it is simply based on a direct comparison between $g(x)$ and $g(x^*)$.*

To characterize the set of global minimizers of (p-RS), we may assume that H is diagonal, i.e.,

$$H = \mathrm{Diag}(\alpha_1, \ldots, \alpha_n), \tag{5}$$

where

$$\alpha_1 = \ldots = \alpha_k < \alpha_{k+1} \leq \ldots \leq \alpha_n$$

and k is the multiplicity of the smallest eigenvalue α_1. Otherwise, let $H = U\Sigma U^T$ be the eigenvalue decomposition of H. Let $y = U^T x$. Then $\|y\| = \|U^T x\| = \|x\|$ and we obtain a diagonal version of (p-RS) in terms of y.

Theorem 2 *The set of global minimizers of (p-RS) is either a singleton or a k-dimensional sphere centered at $(0, \cdots, 0, -\frac{c_{k+1}}{\alpha_{k+1}-\alpha_1}, \cdots, -\frac{c_n}{\sigma_n - \sigma_1})$ with the radius $\sqrt{\left(\frac{\alpha_1}{\sigma}\right)^{\frac{2}{p-2}} - \sum_{i=k+1}^{n} \frac{c_i^2}{(\alpha_i - \alpha_1)^2}}$.*

Proof Let x^* be any global minimizer of (p-RS) and define $t^* = \|x^*\|^{p-2} \geq 0$. Notice that t^* is independent of the choice of x^* since the ℓ_2 norms of all the global minimizers are equal. By Theorem 1, $\alpha_i + \sigma t^* \geq 0$, $\forall i = 1, 2, \ldots, n$. That is, $t^* \in (\max\{-\frac{\alpha_1}{\sigma}, 0\}, +\infty)$. Moreover, the solutions x^* satisfying $(H + \sigma t^* I)x^* = -c$ define the set of the global minimizers. If $H + \sigma t^* I$ is invertible, the global minimizer x^* is uniquely defined by (the still unknown t^* that)

$$x_i^* = \frac{-c_i}{\alpha_i + \sigma t^*}, \; i = 1, \ldots, n.$$

By summing all $(x_i^*)^2$, t^* is necessarily a nonnegative root of the following secular function on a specific open interval:

$$h(t) = \sum_{i=1}^{n} \frac{c_i^2}{(\alpha_i + \sigma t)^2} - t^{\frac{2}{p-2}}, \; t \in I_g = \left(\max\{-\frac{\alpha_1}{\sigma}, 0\}, +\infty\right). \tag{6}$$

Since $\lim_{t\to\max\{-\frac{\alpha_1}{\sigma},0\}} h(t) > 0$, $\lim_{t\to+\infty} h(t) = -\infty$ and $h(t)$ is strictly decreasing on I_g, the secular function $h(t)$ has a unique root on I_g, which must be t^*.

On the other hand, $H + \sigma t^* I$ is singular in which case $t^* = \frac{-\alpha_1}{\sigma}$. (Obviously, this case can not happen for $\alpha_1 > 0$.) Then, $c_1^2 + \ldots + c_k^2 = 0$, and $\alpha_i + \sigma t^* > 0$, $i = k+1, k+2, \ldots, n$ such that

$$\hat{x}^* = \left(0, 0, \ldots, 0, \frac{-c_{k+1}}{\alpha_{k+1} - \alpha_1}, \ldots, \frac{-c_n}{\alpha_n - \alpha_1}\right)^T \tag{7}$$

is one trivial solution to $(H - \alpha_1 I)x^* = -c$. By summing all $(\hat{x}_i^*)^2$ in (7), we again obtain a secular function

$$\hat{h}(t) = \sum_{i=k+1}^{n} \frac{c_i^2}{(\alpha_i + \sigma t)^2} - t^{\frac{2}{p-2}}, \ t \in I_{\hat{g}} = \left[-\frac{\alpha_1}{\sigma}, +\infty\right). \tag{8}$$

Notice that $\hat{h}(t)$ is also strictly decreasing on $I_{\hat{g}}$ and $\lim_{t\to+\infty} \hat{h}(t) = -\infty$. If $\hat{h}\left(-\frac{\alpha_1}{\sigma}\right) = 0$, then $t^* = \frac{-\alpha_1}{\sigma}$ is the unique root of $\hat{h}(t)$ on $I_{\hat{g}}$. Thus, $\hat{x}^*$ defined by (7) is the unique global minimizer of (p-RS).

If $\hat{h}\left(-\frac{\alpha_1}{\sigma}\right) < 0$, then (8) has no solution and the trivial solution $\hat{x}^*$ to $(H - \alpha_1 I)x^* = -c$ does not satisfy $t^* = \frac{-\alpha_1}{\sigma} = \|\hat{x}^*\|^{p-2}$. Then, any x^* satisfying

$$(x_1^*)^2 + \ldots + (x_k^*)^2 + \sum_{i=k+1}^{n} \frac{c_i^2}{(\alpha_i - \alpha_1)^2} = \left(\frac{-\alpha_1}{\sigma}\right)^{\frac{2}{p-2}} \tag{9}$$

is a global minimizer of (p-RS). Namely, the global minimum solution set forms a k-dimensional sphere centered at $(0, \cdots, 0, -\frac{c_{k+1}}{\alpha_{k+1}-\alpha_1}, \cdots, -\frac{c_n}{\sigma_n - \sigma_1})$ with the radius

$$\sqrt{\left(\frac{\alpha_1}{\sigma}\right)^{\frac{2}{p-2}} - \sum_{i=k+1}^{n} \frac{c_i^2}{(\alpha_i - \alpha_1)^2}}.$$

Otherwise, $\hat{h}\left(-\frac{\alpha_1}{\sigma}\right) > 0$, then (8) has no solution and (9) cannot hold for any x^*. We obtain a contradiction that (p-RS) has no global minimizer. The proof is thus complete.

Finally, we show that (p-RS) possesses some hidden convexity that its global minimizer can be obtained by solving an equivalently reformulated convex programming. We first have

Proposition 1 *Suppose H is diagonal. Let x^* be any global minimizer of (p-RS), then*

$$c_i x_i^* \leq 0, \ i = 1, \dots, n.$$

Proof Comparing x^* with $\widetilde{x} = (-x_1^*, x_2^*, x_3^*, \dots, x_n^*)$, we immediately have

$$0 \geq g(x^*) - g(\widetilde{x}) = c_1(x_1^* - \widetilde{x}_1) = 2c_1 x_1^*.$$

A similar argument applying to all other components yields the result. This completes the proof.

By Proposition 1, (p-RS) and (10) below share the same optimal solution set.

$$\begin{array}{ll} \min & \sum_{i=1}^{n} \{ \frac{\alpha_i}{2} x_i^2 + c_i x_i \} + \frac{\sigma}{p} \left(\sum_{i=1}^{n} x_i^2 \right)^{\frac{p}{2}} \\ \text{s. t.} & c_i x_i \leq 0, \quad i = 1, \dots, n. \end{array} \tag{10}$$

Introducing the nonlinear one-to-one map:

$$x_i = \begin{cases} \sqrt{z_i}, & \text{if } c_i \leq 0, \\ -\sqrt{z_i}, & \text{if } c_i > 0, \end{cases} \quad i = 1, \dots, n, \tag{11}$$

the problem (10) becomes the following convex program:

$$\begin{array}{ll} \min & -\sum_{i=1}^{n} |c_i| \sqrt{z_i} + \frac{1}{2} \sum_{i=1}^{n} \alpha_i z_i + \frac{\sigma}{p} \left(\sum_{i=1}^{n} z_i \right)^{\frac{p}{2}} \\ \text{s. t.} & z_i \geq 0, \ i = 1, \dots, n. \end{array} \tag{12}$$

The global optimal solution of (12) can be converted to generate x^* through the transformation (11).

Remark 2 *The first two derivatives of the secular function $h(t)$ are*

$$h'(t) = \sum_{i=1}^{n} \frac{-2\sigma c_i^2}{(\alpha_i + \sigma t)^3} - \frac{2}{p-2} t^{\frac{4-p}{p-2}}$$

and

$$h''(t) = \sum_{i=1}^{n} \frac{6\sigma^2 c_i^2}{(\alpha_i + \sigma t)^4} - \frac{2(4-p)}{(p-2)^2} t^{\frac{6-2p}{p-2}}.$$

$h(t)$ is strictly decreasing on I_g and convex only for $p \geq 4$. For $p = 3$, if $H \not\succeq 0$ (which ensures that $c \neq 0$) and h is restricted to a finite subinterval of I_g covering t^*, by properly choosing the regularization parameter σ, $h(t)$ can be made convex. Notice that the secular function for (TRS) is always convex though.

3 Conclusions

Since the cubic regularization subproblem can be used to modify Newton's method for solving unconstrained optimization problems, it is generally believed that the cubic regularization subproblem is very close to (TRS) in spirit. Our comprehensive analysis on the p-regularized subproblems for general $p > 2$ gives the most detailed comparison between the two types of subproblems and confirms that they do share many similar features.

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