

Cubic regularization of a Newton scheme and its global performance

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Abstract

In this paper we suggest a cubic regularization for a Newton method as applied to unconstrained minimization problem. For this scheme we prove general convergence results. We analyze the behavior of this scheme on different problem classes, for which we get global and local worst-case complexity bounds. It is shown that the search direction can be computed by a standard linear algebra technique.

Keywords: General nonlinear optimization, unconstrained optimization, Newton method, trust-region methods, global complexity bounds, global rate of convergence.

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1 Introduction

Motivation. Starting from the seminal papers by Bennet[1] and Kantorovich [6], the Newton method turned into an important tool for numerous applied problems. In the simplest case of unconstrained minimization of a multivariate function,

$$\min_{x \in R^n} f(x),$$

the standard Newton scheme looks as follows:

$$x_{k+1} = x_k - [f''(x_k)]^{-1} f'(x_k).$$

Despite to its very natural motivation, this scheme has several hidden drawbacks. First of all, it may happen that at current test point the Hessian is degenerate; in this case the method is not well-defined. Secondly, it may happen that this scheme diverges or converges to a saddle point or even to a point of local maximum. In last fifty years the number of different suggestions for improving the scheme was extremely large. The reader can consult a 1000-item bibliography in the recent exhaustive covering of the field [2]. However, all of them combine in one way or another the following elements.

- *Levenberg-Marquardt regularization.* As suggested in [7, 8], if $f''(x)$ is not positive definite, let us regularize it with a unit matrix. Namely, use $d = -G^{-1} f'(x)$ with $G = f''(x) + \gamma I \succ 0$ as a search direction. This strategy sometimes is considered as a way to mix Newton's method with the gradient method.
- *Line search.* Since we are interested in a minimization, it looks reasonable to allow a certain step size $h_k > 0$:

$$x_{k+1} = x_k - h_k [f''(x_k)]^{-1} f'(x_k),$$

(this is a *damped* Newton method [12]). This can help to form a monotone sequence of function values: $f(x_{k+1}) \leq f(x_k)$.

- *Trust-region approach* [5, 4, 3, 2]. In accordance to this approach, at point x_k we have to form a trust region $\Delta(x_k)$. Then the next point x_{k+1} is chosen as a solution to the following auxiliary problem:

$$\min_{x \in \Delta(x_k)} [\langle f'(x_k), x - x_k \rangle + \frac{1}{2} \langle f''(x_k)(x - x_k), x - x_k \rangle].$$

Note that for $\Delta(x_k) \equiv R^n$, this is exactly the standard Newton step.

We would encourage a reader to look in [2] for different combinations and implementations of the above ideas. Here we only mention that despite to a huge variety of results, there still exist open questions in this field. And, in our opinion, the most important questions are related to the global behavior of Newton-type schemes.

Indeed, as far as we know, up to now there are *absolutely no results* on the global performance of Newton method. Even for an easy class of smooth strongly convex functions we can get a rate of convergence for a damped Newton method only by arguing that it is not much worse than the gradient method. In fact, up to now the relations between the gradient method and the Newton method have not been clarified. Quite often one reads

opinion that the Newton method is good at the final stage of the minimization process, but it is better to use the gradient method for the first iterations. Here we dispute this position: we show that theoretically, a properly chosen Newton-type scheme *outperforms* the gradient scheme *in all known* situations.

In this paper we propose a modification of Newton method, which is constructed in a similar way to the well-known *gradient mapping* [9]. Assume that function f has a Lipschitz continuous gradient:

$$\|f'(x) - f'(y)\| \leq D\|y - x\|, \quad \forall x, y \in R^n.$$

Suppose we need to solve the problem

$$\min_{x \in Q} f(x),$$

where Q is a closed convex set. Then we can choose the next point x_{k+1} in our sequence as a solution of the following auxiliary problem:

$$\min_{y \in Q} \xi_{1,x_k}(y), \quad \xi_{1,x_k}(y) = f(x_k) + \langle f'(x_k), y - x_k \rangle + \frac{1}{2}D\|y - x_k\|^2. \quad (1.1)$$

The convergence of this scheme follows from the fact that $\xi_{1,x_k}(y)$ is an *upper first-order* approximation of the objective function (see, for example, [10], Section 2.2.4, for details). If $Q \equiv R^n$, then the rule (1.1) results in a usual gradient scheme:

$$x_{k+1} = x_k - \frac{1}{D}f'(x_k).$$

Note that we can do similar thing with the second-order approximation. Indeed, assume that the Hessian of our objective function is Lipschitz continuous:

$$\|f''(x) - f''(y)\| \leq L\|x - y\|, \quad \forall x, y \in R^n.$$

Then it is easy to see that the auxiliary function

$$\xi_{2,x}(y) = f(x) + \langle f'(x), y - x \rangle + \frac{1}{2}\langle f''(x)(y - x), y - x \rangle + \frac{L}{6}\|y - x\|^3$$

will be an *upper second-order* approximation for our objective function:

$$f(y) \leq \xi_{2,x}(y) \quad \forall y \in R^n.$$

Thus, we can try to find the next point in our second-order scheme from the following auxiliary minimization problem:

$$x_{k+1} \in \text{Arg min}_y \xi_{2,x_k}(y). \quad (1.2)$$

This is exactly the approach we analyze in this paper; we call it *cubic regularization* of Newton's method. Note that problem (1.2) is non-convex and it can have local minima. However, our approach is implementable since this problem is equivalent to minimizing an explicitly written *convex function* of one variable.

Contents. In Section 2 we introduce cubic regularization and present its main properties. In Section 3 we analyze the general convergence of the process. We prove that under very

mild assumptions all limit points of the process satisfy necessary second-order optimality condition. Moreover, it appears that the process cannot be attracted by a non-degenerate saddle point. In this general setting we get a rate of convergence for the norms of the gradients, which is better than the rate ensured by the gradient scheme. We prove also the local quadratic convergence of the process. In Section 4 we give the global complexity results of our scheme for different problem classes. We show that in all situations the global rate of convergence is surprisingly fast (like $O(\frac{1}{k^2})$ for star-convex functions, where k is the iteration counter). Moreover, under rather weak non-degeneracy assumptions, we have local super-linear convergence either of the order $\frac{4}{3}$ or $\frac{3}{2}$. We show that this happens even if the Hessian is degenerate at the solution set. In Section 5 we show how to compute a solution to the cubic regularization problem and discuss some efficient strategies for estimating the Lipschitz constant for the Hessian. We conclude the paper by a short discussion presented in Section 6.

Notation. In what follows we denote by $\langle \cdot, \cdot \rangle$ the standard inner product in R^n :

$$\langle x, y \rangle = \sum_{i=1}^n x^{(i)} y^{(i)}, \quad x, y \in R^n,$$

and by $\|x\|$ the standard Euclidean norm:

$$\|x\| = \langle x, x \rangle^{1/2}.$$

For a symmetric $n \times n$ matrix H , its spectrum is denoted by $\{\lambda_i(H)\}_{i=1}^n$. We assume that the eigenvalues are numbered in decreasing order:

$$\lambda_1(H) \geq \dots \geq \lambda_n(H).$$

Hence, we write $H \succeq 0$ if and only if $\lambda_n(H) \geq 0$. In what follows, for a matrix A we use the standard spectral matrix norm:

$$\|A\| = \lambda_1(AA^T)^{1/2}.$$

Finally, I denotes a unit $n \times n$ matrix.

2 Cubic regularization of quadratic approximation

Let $\mathcal{F} \subseteq R^n$ be a closed convex set with non-empty interior. Consider a twice differentiable function $f(x)$, $x \in \mathcal{F}$. Let $x_0 \in \text{int } \mathcal{F}$ be a starting point of our iterative schemes. We assume that the set \mathcal{F} is large enough: It contains at least the level set

$$\mathcal{L}(f(x_0)) \equiv \{x \in R^n : f(x) \leq f(x_0)\}$$

in its interior. Moreover, in this paper we always assume the following.

Assumption 1 *The Hessian of function f is Lipschitz continuous on \mathcal{F} :*

$$\|f''(x) - f''(y)\| \leq L\|x - y\|, \quad \forall x, y \in \mathcal{F}. \quad (2.1)$$

for some $L > 0$.

For the sake of completeness, let us present the following trivial consequences of our assumption (compare [12, Section 3]).

Lemma 1 *For any x and y from \mathcal{F} we have*

$$\|f'(y) - f'(x) - f''(x)(y - x)\| \leq \frac{1}{2}L\|y - x\|^2, \quad (2.2)$$

$$|f(y) - f(x) - \langle f'(x), y - x \rangle - \frac{1}{2}\langle f''(x)(y - x), y - x \rangle| \leq \frac{L}{6}\|y - x\|^3. \quad (2.3)$$

Proof:

Indeed,

$$\begin{aligned} \|f'(y) - f'(x) - f''(x)(y - x)\| &= \left\| \int_0^1 [f''(x + \tau(y - x)) - f''(x)](y - x) d\tau \right\| \\ &\leq L\|y - x\|^2 \int_0^1 \tau d\tau = \frac{1}{2}L\|y - x\|^2. \end{aligned}$$

Therefore,

$$\begin{aligned} &|f(y) - f(x) - \langle f'(x), y - x \rangle - \frac{1}{2}\langle f''(x)(y - x), y - x \rangle| \\ &= \left| \int_0^1 \langle f'(x + \lambda(y - x)) - f'(x) - \lambda f''(x)(y - x), y - x \rangle d\lambda \right| \\ &\leq \frac{1}{2}L\|y - x\|^3 \int_0^1 \lambda^2 d\lambda = \frac{L}{6}\|y - x\|^3. \end{aligned}$$

□

Let M be a positive parameter. Define a modified Newton step using the following *cubic regularization* of the quadratic approximation of function $f(x)$:

$$T_M(x) \in \operatorname{Arg\,min}_y \left[\langle f'(x), y - x \rangle + \frac{1}{2}\langle f''(x)(y - x), y - x \rangle + \frac{M}{6}\|y - x\|^3 \right], \quad (2.4)$$

where "Arg" indicates that $T_M(x)$ is chosen from the set of global minima of the corresponding minimization problem. We postpone discussion of the complexity of finding this point up to Section 5.1.

Note that the point $T_M(x)$ satisfies the following system of nonlinear equations:

$$f'(x) + f''(x)(y - x) + \frac{1}{2}M\|y - x\| \cdot (y - x) = 0. \quad (2.5)$$

Denote $r_M(x) = \|x - T_M(x)\|$. Taking in (2.5) $y = T_M(x)$ and multiplying it by $T_M(x) - x$ we get the following equation:

$$\langle f'(x), T_M(x) - x \rangle + \langle f''(x)(T_M(x) - x), T_M(x) - x \rangle + \frac{1}{2}Mr_M^3(x) = 0. \quad (2.6)$$

In our analysis of the process (3.3), we also need the following fact.

Proposition 1 *For any $x \in \mathcal{F}$ we have*

$$f''(x) + \frac{1}{2}Mr_M(x)I \succeq 0. \quad (2.7)$$

This statement follows from Theorem 10, which will be proved later in Section 5.1. Now let us present the main properties of the mapping $T_M(A)$.

Lemma 2 *For any $x \in \mathcal{F}$, $f(x) \leq f(x_0)$, we have the following relation:*

$$\langle f'(x), x - T_M(x) \rangle \geq 0. \quad (2.8)$$

If $M \geq \frac{2}{3}L$ and $x \in \text{int } \mathcal{F}$, then $T_M(x) \in \mathcal{L}(f(x)) \subseteq \mathcal{F}$.

Proof:

Indeed, multiplying (2.7) by $x - T_M(x)$ twice, we get

$$\langle f''(x)(T_M(x) - x), T_M(x) - x \rangle + \frac{1}{2}Mr_M^3(x) \geq 0.$$

Therefore (2.8) follows from (2.6).

Further, let $M \geq \frac{2}{3}L$. Assume that $T_M(x) \notin \mathcal{F}$. Then $r_M(x) > 0$. Consider the following points:

$$y(\alpha) = x + \alpha(T_M(x) - x), \quad \alpha \in [0, 1].$$

Since $y(0) \in \text{int } \mathcal{F}$, the value

$$\bar{\alpha} : y(\bar{\alpha}) \in \partial \mathcal{F}$$

is well defined. In accordance to our assumption, $\bar{\alpha} < 1$ and $y(\alpha) \in \mathcal{F}$ for all $\alpha \in [0, \bar{\alpha}]$. Therefore, using (2.3), relation (2.6) and inequality (2.8), we get the following:

$$\begin{aligned} f(y(\alpha)) &\leq f(x) + \langle f'(x), y(\alpha) - x \rangle + \frac{1}{2}\langle f''(x)(y(\alpha) - x), y(\alpha) - x \rangle + \frac{\alpha^3 L}{6}r_M^3(x) \\ &\leq f(x) + \langle f'(x), y(\alpha) - x \rangle + \frac{1}{2}\langle f''(x)(y(\alpha) - x), y(\alpha) - x \rangle + \frac{\alpha^3 M}{4}r_M^3(x) \\ &= f(x) + (\alpha - \frac{\alpha^2}{2})\langle f'(x), T_M(x) - x \rangle - \frac{\alpha^2(1-\alpha)}{4}Mr_M^3(x) \\ &\leq f(x) - \frac{\alpha^2(1-\alpha)}{4}Mr_M^3(x). \end{aligned}$$

Thus, $f(y(\bar{\alpha})) < f(x)$. Therefore $y(\bar{\alpha}) \in \text{int } \mathcal{L}(f(x)) \subseteq \text{int } \mathcal{F}$. That is a contradiction. Hence, $T_M(x) \in \mathcal{F}$ and using the same arguments we prove that $f(T_M(x)) \leq f(x)$. \square

Lemma 3 *If $T_M(x) \in \mathcal{F}$ then*

$$\|f'(T_M(x))\| \leq \frac{1}{2}(L + M)r_M^2(x). \quad (2.9)$$

Proof:

From the equation (2.5) we get

$$\|f'(x) + f''(x)(T_M(x) - x)\| = \frac{1}{2}Mr_M^2(x).$$

On the other hand, in view of (2.2), we have

$$\|f'(T_M(x)) - f'(x) - f''(x)(T_M(x) - x)\| \leq \frac{1}{2}Lr_M^2(x).$$

Combining these two relations, we obtain inequality (2.9). \square

Define

$$\bar{f}_M(x) = \min_y \left[f(x) + \langle f'(x), y - x \rangle + \frac{1}{2} \langle f''(x)(y - x), y - x \rangle + \frac{M}{6} \|y - x\|^3 \right].$$

Lemma 4 For any $x \in \mathcal{F}$ we have

$$\bar{f}_M(x) \leq \min_{y \in \mathcal{F}} \left[f(y) + \frac{L+M}{6} \|y - x\|^3 \right], \quad (2.10)$$

$$f(x) - \bar{f}_M(x) \geq \frac{M}{12} r_M^3(x). \quad (2.11)$$

Moreover, if $M \geq L$, then $T_M(x) \in \mathcal{F}$ and

$$f(T_M(x)) \leq \bar{f}_M(x). \quad (2.12)$$

Proof:

Indeed, using the lower bound in (2.3), for any $y \in \mathcal{F}$ we have

$$f(x) + \langle f'(x), y - x \rangle + \frac{1}{2} \langle f''(x)(y - x), y - x \rangle \leq f(y) + \frac{L}{6} \|y - x\|^3.$$

and inequality in (2.10) follows from the definition of $\bar{f}_M(x)$.

Further, in view of definition of the point $T_M(x)$, relation (2.6) and inequality (2.8), we have

$$\begin{aligned} f(x) - \bar{f}_M(x) &= \langle f'(x), x - T_M(x) \rangle - \frac{1}{2} \langle f''(x)(T_M(x) - x), T_M(x) - x \rangle - \frac{M}{6} r_M^3(x) \\ &= \frac{1}{2} \langle f'(x), x - T_M(x) \rangle + \frac{M}{12} r_M^3(x) \geq \frac{M}{12} r_M^3(x). \end{aligned}$$

Finally, if $M \geq L$, then $T_M(x) \in \mathcal{F}$ in view of Lemma 2. Therefore we get inequality (2.12) from the upper bound in (2.3). \square

3 General convergence results

In this paper the main problem of interest is:

$$\min_{x \in R^n} f(x), \quad (3.1)$$

where the objective function $f(x)$ satisfies Assumption 1. Recall that the necessary conditions for a point x^* to be a local solution to problem (3.1) are as follows:

$$f'(x^*) = 0, \quad f''(x^*) \succeq 0. \quad (3.2)$$

Therefore, for an arbitrary $x \in \mathcal{F}$ we can introduce the following measure of local optimality:

$$\mu_M(x) = \max \left\{ \sqrt{\frac{2}{L+M} \|f'(x)\|}, -\frac{2}{2L+M} \lambda_n(f''(x)) \right\},$$

where M is a positive parameter. It is clear that for any x from \mathcal{F} the measure $\mu_M(x)$ is non-negative and it vanishes only at the points satisfying conditions (3.2). The analytical form of this measure can be justified by the following result.

Lemma 5 For any $x \in \mathcal{F}$ we have $\mu_M(T_M(x)) \leq r_M(x)$.

Proof:

The proof follows immediately from inequality (2.9) and the relation (2.7) since

$$f''(T_M(x)) \geq f''(x) - Lr_M(x)I \geq -(\frac{1}{2}M + L)r_M(x)I.$$

□

Let $L_0 \in (0, L]$ be a positive parameter. Consider the following regularized Newton scheme.

Cubic regularization of Newton method	
Initialization: Choose $x_0 \in R^n$.	
Iteration k, ($k \geq 0$): <ol style="list-style-type: none"> 1. Find $M_k \in [L_0, 2L]$ such that $f(T_{M_k}(x_k)) \leq \bar{f}_{M_k}(x_k)$. 2. Set $x_{k+1} = T_{M_k}(x_k)$. 	(3.3)

Since $\bar{f}_M(x) \leq f(x)$, this process is monotone:

$$f(x_{k+1}) \leq f(x_k).$$

If the constant L is known, we can take $M_k \equiv L$ in Step 1 of this scheme. In the opposite case, it is possible to apply a simple search procedure; we will discuss its complexity later in Section 5.2. Now let us make the following simple observation.

Theorem 1 Let the sequence $\{x_i\}$ be generated by method (3.3). Assume that the objective function $f(x)$ is bounded below:

$$f(x) \geq f^* \quad \forall x \in \mathcal{F}.$$

Then $\sum_{i=0}^{\infty} r_{M_i}^3(x_i) \leq \frac{12}{L_0}(f(x_0) - f^*)$. Moreover, $\lim_{i \rightarrow \infty} \mu_L(x_i) = 0$ and for any $k \geq 1$ we have

$$\min_{1 \leq i \leq k} \mu_L(x_i) \leq \frac{8}{3} \cdot \left(\frac{3(f(x_0) - f^*)}{2k \cdot L_0} \right)^{1/3}. \quad (3.4)$$

Proof:

In view of inequality (2.11) we have

$$f(x_0) - f^* \geq \sum_{i=0}^{k-1} [f(x_i) - f(x_{i+1})] \geq \sum_{i=0}^{k-1} \frac{M_i}{12} r_{M_i}^3(x_i) \geq \frac{L_0}{12} r_{M_i}^3(x_i).$$

It remains to use the statement of Lemma 5 and the upper bound on M_k in (3.3):

$$r_{M_i}(x_i) \geq \mu_{M_i}(x_{i+1}) \geq \frac{3}{4}\mu_L(x_{i+1}).$$

□

Note that inequality (3.4) implies that

$$\min_{1 \leq i \leq k} \|f'(x_i)\| \leq O(k^{-2/3}).$$

It is well known that for gradient scheme a possible level of the right-hand side in this inequality is of the order $O(k^{-1/2})$ (see, for example, [10], inequality (1.2.13)).

Theorem 1 helps to get the convergence results in many different situations. We mention only one of such possibilities.

Theorem 2 *Let sequence $\{x_i\}$ be generated by method (3.3). Assume that for some $i \geq 0$ the set $\mathcal{L}(f(x_i))$ be bounded. Then there exists a limit*

$$\lim_{i \rightarrow \infty} f(x_i) = f^*.$$

The set X^ of the limit points of this sequence is non-empty. Moreover, this is a connected set, such that for any $x^* \in X^*$ we have*

$$f(x^*) = f^*, \quad f'(x^*) = 0, \quad f''(x^*) \succeq 0.$$

Proof:

The proof of this theorem can be derived from Theorem 1 in a standard way. □

Let us describe now the behavior of the process (3.3) in a neighborhood of a non-degenerate stationary point, which is not a minimum point.

Lemma 6 *Let $\bar{x} \in \text{int } \mathcal{F}$ be a non-degenerate saddle point or maximum point of function $f(x)$:*

$$f'(\bar{x}) = 0, \quad \lambda_n(f''(\bar{x})) < 0.$$

Then there exist constants $\epsilon, \delta > 0$ such that whenever a point x_i appears to be in a dangerous neighborhood of stationary point \bar{x} :

$$\|x_i - \bar{x}\| \leq \epsilon, \quad f(x_i) \geq f(\bar{x}),$$

the next point x_{i+1} leaves the neighborhood:

$$f(x_{i+1}) \leq f(\bar{x}) - \delta.$$

Hence, the process (3.3) can only escape from the neighborhood of point \bar{x} .

Proof:

Let for some d with $\|d\| = 1$ and for some $\bar{\tau} > 0$ we have

$$\langle f''(\bar{x})d, d \rangle \equiv -\sigma < 0, \quad \bar{x} \pm \bar{\tau}d \in \mathcal{F}.$$

Define $\epsilon = \min\{\frac{\sigma}{2L}, \bar{\tau}\}$ and $\delta = \frac{\sigma}{6}\epsilon^2$. Then in view of inequality (2.10), upper bound on M_i and inequality (2.3), for $|\tau| \leq \bar{\tau}$ we get the following estimate

$$\begin{aligned} f(x_{i+1}) &\leq f(\bar{x} + \tau d) + \frac{L}{2}\|\bar{x} + \tau d - x_i\|^3 \\ &\leq f(\bar{x}) - \sigma\tau^2 + \frac{L}{6}|\tau|^3 + \frac{L}{2}[\epsilon^2 + 2\tau\langle d, \bar{x} - x_i \rangle + \tau^2]^{3/2}. \end{aligned}$$

Since we are free in the choice of the sign of τ , we can guarantee that

$$f(x_{i+1}) \leq f(\bar{x}) - \sigma\tau^2 + \frac{L}{6}|\tau|^3 + \frac{L}{2}[\epsilon^2 + \tau^2]^{3/2}, \quad |\tau| \leq \bar{\tau}.$$

Let us choose $\tau = \epsilon \leq \bar{\tau}$. Then

$$f(x_{i+1}) \leq f(\bar{x}) - \sigma\tau^2 + \frac{5L}{3}\tau^3 \leq f(\bar{x}) - \sigma\tau^2 + \frac{5L}{3} \cdot \frac{\sigma}{2L} \cdot \tau^2 = f(\bar{x}) - \frac{1}{6}\sigma\tau^2.$$

Since the process (3.3) is monotone in the objective function, it will never come again in a dangerous neighborhood of the point \bar{x} . \square

Note that the above theorem works even if $x_i = \bar{x}$ and $f'(x_i) = 0$.

Consider now the behavior of the regularized Newton scheme (3.3) in a neighborhood of a non-degenerate local minimum. It appears that in such a situation assumption $L_0 > 0$ is not necessary anymore. Let us analyze a relaxed version of (3.3):

$$\boxed{x_{k+1} = T_{M_k}(x_k), \quad k \geq 0} \tag{3.5}$$

where $M_k \in (0, 2L]$. Denote

$$\delta_k = \frac{L\|f'(x_k)\|}{\lambda_n^2(f''(x_k))}.$$

Theorem 3 *Let $f''(x_0) \succ 0$. Assume that δ_0 is small enough: $\delta_0 \leq \frac{1}{4}$. And let points $\{x_k\}$ be generated by (3.5). Then:*

1. *For all $k \geq 0$ the values δ_k are well defined and they converge quadratically to zero:*

$$\delta_{k+1} \leq \frac{3}{2} \left(\frac{\delta_k}{1-\delta_k} \right)^2 \leq \frac{2}{3}\delta_k, \quad k \geq 0. \tag{3.6}$$

2. *Minimal eigenvalues of all Hessians $f''(x_k)$ lie within the following bounds:*

$$e^{-1}\lambda_n(f''(x_0)) \leq \lambda_n(f''(x_k)) \leq e^{3/4}\lambda_n(f''(x_0)). \tag{3.7}$$

3. *The whole sequence $\{x_i\}$ converges quadratically to a point x^* , which is a non-degenerate local minimum of function $f(x)$. In particular, for any $k \geq 1$ we have*

$$\|f'(x_k)\| \leq \lambda_n^2(f''(x_0)) \frac{9e^{3/2}}{16L} \left(\frac{1}{2} \right)^{2^k}. \tag{3.8}$$

Proof:

Assume that for some $k \geq 0$ we have $f''(x_k) \succ 0$. Then the corresponding δ_k is well defined. Assume that $\delta_k \leq \frac{1}{4}$. From equation (2.5) we have

$$r_{M_k}(x_k) = \|T_{M_k}(x_k) - x_k\| = \|(f''(x_k) + r_{M_k}(x_k)\frac{M_k}{2}I)^{-1}f'(x_k)\| \leq \frac{\|f'(x_k)\|}{\lambda_n(f''(x_k))}. \quad (3.9)$$

Note also that $f''(x_{k+1}) \succeq f''(x_k) - r_{M_k}(x_k)LI$. Therefore

$$\begin{aligned} \lambda_n(f''(x_{k+1})) &\geq \lambda_n(f''(x_k)) - r_{M_k}(x_k)L \\ &\geq \lambda_n(f''(x_k)) - \frac{L\|f'(x_k)\|}{\lambda_n(f''(x_k))} = (1 - \delta_k)\lambda_n(f''(x_k)). \end{aligned}$$

Thus, $f''(x_{k+1})$ is also positive definite. Moreover, using inequality (2.9) and the upper bound for M_k we obtain

$$\delta_{k+1} = \frac{L\|f'(x_{k+1})\|}{\lambda_n(f''(x_{k+1}))} \leq \frac{3L^2r_{M_k}^2(x_k)}{2\lambda_n^2(f''(x_{k+1}))} \leq \frac{3L^2\|f'(x_k)\|^2}{2\lambda_n^4(f''(x_k))(1-\delta_k)^2} = \frac{3}{2} \left(\frac{\delta_k}{1-\delta_k} \right)^2 \leq \frac{2}{3}\delta_k.$$

Thus, $\delta_{k+1} \leq \frac{1}{4}$ and we prove (3.6) by induction.

Further, as we have already seen,

$$\ln \frac{\lambda_n(f''(x_k))}{\lambda_n(f''(x_0))} \geq \sum_{i=0}^{\infty} \ln(1 - \delta_i) \geq - \sum_{i=0}^{\infty} \frac{\delta_i}{1-\delta_i} \geq -\frac{1}{1-\delta_0} \sum_{i=0}^{\infty} \delta_i \geq -1.$$

In order to get an upper bound, note that $f''(x_{k+1}) \preceq f''(x_k) + r_{M_k}(x_k)LI$. Hence,

$$\lambda_n(f''(x_{k+1})) \leq \lambda_n(f''(x_k)) + r_{M_k}(x_k)L \leq (1 + \delta_k)\lambda_n(f''(x_k)).$$

Therefore

$$\ln \frac{\lambda_n(f''(x_k))}{\lambda_n(f''(x_0))} \leq \sum_{i=0}^{\infty} \ln(1 + \delta_i) \leq \sum_{i=0}^{\infty} \delta_i \leq \frac{3}{4}.$$

It remains to prove Item 3 of the theorem. In view of inequalities (3.9) and (3.7) we have

$$r_{M_k}(x_k) \leq \frac{1}{L}\lambda_n(f''(x_k))\delta_k \leq \frac{e^{3/4}}{L}\lambda_n(f''(x_0))\delta_k.$$

Thus, $\{x_i\}$ is a Cauchy sequence, which has a unique limit point x^* . Since the eigenvalues of $f''(x)$ are continuous functions of x , from (3.7) we conclude that $f''(x^*) > 0$.

Further, from inequality (3.6) we get

$$\delta_{k+1} \leq \frac{\delta_k^2}{(1-\delta_0)^2} \leq \frac{16}{9}\delta_k^2.$$

Denoting $\hat{\delta}_k = \frac{16}{9}\delta_k$, we get $\hat{\delta}_{k+1} \leq \hat{\delta}_k^2$. Thus, for any $k \geq 1$ we have

$$\delta_k = \frac{9}{16}\hat{\delta}_k \leq \frac{9}{16}\hat{\delta}_0^{2^k} < \frac{9}{16} \left(\frac{1}{2} \right)^{2^k}.$$

Using the upper bound in (3.7), we get (3.8). \square

4 Global efficiency on specific problem classes

In the previous section we have already seen that the modified Newton scheme can be supported by a global efficiency estimate (3.4) on a general class of non-convex problems. The main goal of this section is to show that on more specific classes of non-convex problems the global performance of the scheme (3.3) is much better. To the best of our knowledge, the results of this section are the first global complexity results on a Newton-type scheme. The nice feature of the scheme (3.3) consists in its ability to adjust the performance to a specific problem class automatically.

4.1 Star-convex functions

Let us start from a definition.

Definition 1 *We call a function $f(x)$ star-convex if its set of global minimums X^* is not empty and for any $x^* \in X^*$ and any $x \in R^n$ we have*

$$f(\alpha x^* + (1 - \alpha)x) \leq \alpha f(x^*) + (1 - \alpha)f(x) \quad \forall x \in \mathcal{F}, \forall \alpha \in [0, 1]. \quad (4.1)$$

A particular example of a star-convex function is a usual convex function. However, in general, a star-convex function does not need to be convex.

Theorem 4 *Assume that the objective function in (3.1) is star-convex and the set \mathcal{F} is bounded: $\text{diam } \mathcal{F} = D < \infty$. Let the sequence $\{x_k\}$ be generated by method (3.3).*

1. *If $f(x_0) - f^* \geq \frac{3}{2}LD^3$, then $f(x_1) - f^* \leq \frac{1}{2}LD^3$.*
2. *If $f(x_0) - f^* \leq \frac{3}{2}LD^3$, then the rate of convergence of the process (3.3) is as follows:*

$$f(x_k) - f(x^*) \leq \frac{3LD^3}{2(1+\frac{1}{3}k)^2}, \quad k \geq 0. \quad (4.2)$$

Proof:

Indeed, in view of inequality (2.10), upper bound on the parameters M_k and definition (4.1), for any $k \geq 0$ we have:

$$\begin{aligned} f(x_{k+1}) - f(x^*) &\leq \min_y \left[f(y) - f(x^*) + \frac{L}{2} \|y - x_k\|^3 : y = \alpha x^* + (1 - \alpha)x_k, \alpha \in [0, 1] \right] \\ &\leq \min_{\alpha \in [0, 1]} \left[f(x_k) - f(x^*) - \alpha(f(x_k) - f(x^*)) + \frac{L}{2} \alpha^3 \|x^* - x_k\|^3 \right] \\ &\leq \min_{\alpha \in [0, 1]} \left[f(x_k) - f(x^*) - \alpha(f(x_k) - f(x^*)) + \frac{L}{2} \alpha^3 D^3 \right]. \end{aligned}$$

The minimum of the objective function in the last minimization problem in $\alpha \geq 0$ is achieved for

$$\alpha_k = \sqrt{\frac{2(f(x_k) - f(x^*))}{3LD^3}}.$$

If $\alpha_k \geq 1$, then the actual optimal value corresponds to $\alpha = 1$. In this case

$$f(x_{k+1}) - f(x^*) \leq \frac{1}{2}LD^3.$$

Since the process (3.3) is monotone, this can happen only at the first iteration of the method.

Assume that $\alpha_k \leq 1$. Then

$$f(x_{k+1}) - f(x^*) \leq f(x_k) - f(x^*) - \left[\frac{2}{3}(f(x_k) - f(x^*)) \right]^{3/2} \frac{1}{\sqrt{LD^3}}.$$

Or, in a more convenient notation, that is $\alpha_{k+1}^2 \leq \alpha_k^2 - \frac{2}{3}\alpha_k^3 < \alpha_k^2$. Therefore

$$\frac{1}{\alpha_{k+1}} - \frac{1}{\alpha_k} = \frac{\alpha_k - \alpha_{k+1}}{\alpha_k \alpha_{k+1}} = \frac{\alpha_k^2 - \alpha_{k+1}^2}{\alpha_k \alpha_{k+1} (\alpha_k + \alpha_{k+1})} \geq \frac{\alpha_k^2 - \alpha_{k+1}^2}{2\alpha_k^3} \geq \frac{1}{3}.$$

Thus, $\frac{1}{\alpha_k} \geq \frac{1}{\alpha_0} + \frac{k}{3} \geq 1 + \frac{k}{3}$, and (4.2) follows. \square

Let us introduce now a generalization of the notion of non-degenerate global minimum.

Definition 2 *We say that the optimal set X^* of function $f(x)$ is globally non-degenerate if there exists a constant $\gamma > 0$ such that for any $x \in \mathcal{F}$ we have*

$$f(x) - f^* \geq \frac{\gamma}{2} \rho^2(x, X^*), \quad (4.3)$$

where f^* is the global minimal value of function $f(x)$, and $\rho(x, X^*)$ is the Euclidean distance from x to X^* .

Of course, this property holds for strongly convex functions (in this case X^* is a singleton), however it can also hold for some non-convex functions. Moreover, if the set X^* has a connected non-trivial component, the Hessians of the objective function at these points *cannot* be non-degenerate. However, as we will see, in this situation the modified Newton scheme ensures a super-linear rate of convergence. Denote

$$\bar{\omega} = \frac{1}{L^2} \left(\frac{\gamma}{2} \right)^3.$$

Theorem 5 *Let function $f(x)$ be star-convex. Assume that it has also a globally non-degenerate optimal set. Then the performance of the scheme (3.3) on this problem is as follows.*

1. *If $f(x_0) - f(x^*) \geq \frac{4}{9}\bar{\omega}$, then at the first phase of the process we get the following rate of convergence:*

$$f(x_k) - f(x^*) \leq \left[(f(x_0) - f(x^*))^{1/4} - \frac{k}{6} \sqrt{\frac{2}{3}} \bar{\omega}^{1/4} \right]^4. \quad (4.4)$$

This phase is terminated as soon as $f(x_{k_0}) - f(x^) \leq \frac{4}{9}\bar{\omega}$ for some $k_0 \geq 0$.*

2. *For $k \geq k_0$ the sequence converges superlinearly:*

$$f(x_{k+1}) - f(x^*) \leq \frac{1}{2} (f(x_k) - f(x^*)) \sqrt{\frac{f(x_k) - f(x^*)}{\bar{\omega}}}. \quad (4.5)$$

Proof:

Denote by x_k^* the projection of the point x_k onto the optimal set X^* . In view of inequality (2.10), upper bound on the parameters M_k and definitions (4.1), (4.3), for any $k \geq 0$ we have:

$$\begin{aligned} f(x_{k+1}) - f(x^*) &\leq \min_{\alpha \in [0,1]} \left[f(x_k) - f(x^*) - \alpha(f(x_k) - f(x^*)) + \frac{L}{2}\alpha^3 \|x_k^* - x_k\|^3 \right] \\ &\leq \min_{\alpha \in [0,1]} \left[f(x_k) - f(x^*) - \alpha(f(x_k) - f(x^*)) + \frac{L}{2}\alpha^3 \left(\frac{2}{\gamma}(f(x_k) - f(x^*)) \right)^{3/2} \right]. \end{aligned}$$

Denoting $\Delta_k = (f(x_k) - f(x^*))/\bar{\omega}$, we get inequality

$$\Delta_{k+1} \leq \min_{\alpha \in [0,1]} \left[\Delta_k - \alpha\Delta_k + \frac{1}{2}\alpha^3 \Delta_k^{3/2} \right]. \quad (4.6)$$

Note that the first order optimality condition for $\alpha \geq 0$ in this problem is

$$\alpha_k = \sqrt{\frac{2}{3}\Delta_k^{-1/2}}.$$

Therefore, if $\Delta_k \geq \frac{4}{9}$, we get

$$\Delta_{k+1} \leq \Delta_k - \left(\frac{2}{3}\right)^{3/2} \Delta_k^{3/4}.$$

Denoting $u_k = \frac{9}{4}\Delta_k$ we get a simpler relation:

$$u_{k+1} \leq u_k - \frac{2}{3}u_k^{3/4},$$

which is applicable if $u_k \geq 1$. Since the right-hand side of this inequality is increasing for $u_k \geq \frac{1}{16}$, let us prove by induction that

$$u_k \leq \left[u_0^{1/4} - \frac{k}{6} \right]^4.$$

Indeed, inequality

$$\left[u_0^{1/4} - \frac{k+1}{6} \right]^4 \geq \left[u_0^{1/4} - \frac{k}{6} \right]^4 - \frac{2}{3} \left[u_0^{1/4} - \frac{k}{6} \right]^3$$

clearly is equivalent to

$$\begin{aligned} \frac{2}{3} \left[u_0^{1/4} - \frac{k}{6} \right]^3 &\geq \left[u_0^{1/4} - \frac{k}{6} \right]^4 - \left[u_0^{1/4} - \frac{k+1}{6} \right]^4 = \frac{1}{6} \left[u_0^{1/4} - \frac{k}{6} \right]^3 \\ &+ \left[u_0^{1/4} - \frac{k}{6} \right]^2 \left[u_0^{1/4} - \frac{k+1}{6} \right] + \left[u_0^{1/4} - \frac{k}{6} \right] \left[u_0^{1/4} - \frac{k+1}{6} \right]^2 + \left[u_0^{1/4} - \frac{k+1}{6} \right]^3, \end{aligned}$$

which is obviously true.

Finally, if $u_k \leq 1$, then the optimal value for α in (4.6) is one and we get (4.5). \square

4.2 Gradient-dominated functions

Let us study now another interesting class of problems.

Definition 3 A function $f(x)$ is called gradient dominated of degree $p \in [1, 2]$ if it attains a global minimum at some point x^* and for any $x \in \mathcal{F}$ we have

$$f(x) - f(x^*) \leq \tau_f \|f'(x)\|^p, \quad (4.7)$$

where τ_f is a positive constant. The parameter p is called the degree of domination.

Note that we do not assume that the global minimum of function f is unique. For $p = 2$ this class of functions has been introduced in [13].

Let us give several examples of gradient dominated functions.

Example 1 *Convex functions.* Let f be convex on R^n . Assume it achieves its minimum at point x^* . Then, for any $x \in R^n$, $\|x - x^*\| \leq R$, we have

$$f(x) - f(x^*) \leq \langle f'(x), x - x^* \rangle \leq \|f'(x)\| \cdot R.$$

Thus, on the set $\mathcal{F} = \{x : \|x - x^*\| \leq R\}$, function f is a gradient dominated function of degree one with $\tau_f = R$. \square

Example 2 *Strongly convex functions.* Let f be differentiable and strongly convex on R^n . This means that there exists a constant $\gamma > 0$ such that

$$f(y) \geq f(x) + \langle f'(x), y - x \rangle + \frac{1}{2}\gamma \|y - x\|^2, \quad (4.8)$$

for all $x, y \in R^n$. Then, (see, for example, [10], inequality (2.1.19)),

$$f(x) - f(x^*) \leq \frac{1}{2\gamma} \|f'(x)\|^2 \quad \forall x \in R^n.$$

Thus, on the set $\mathcal{F} = R^n$, function f is a gradient dominated function of degree two with $\tau_f = \frac{1}{2\gamma}$. \square

Example 3 *Sum of squares.* Consider a system of non-linear equations:

$$g(x) = 0 \quad (4.9)$$

where $g(x) = (g_1(x), \dots, g_m(x))^T : R^n \rightarrow R^m$ is a differentiable function. We assume that $m \leq n$ and that there exists a solution x^* to (4.9). Let us assume in addition that the Jacobian

$$J(x) = (g'_1(x), \dots, g'_m(x))$$

is uniformly non-degenerate on a certain convex set \mathcal{F} containing x^* . This means that the value

$$\sigma \equiv \inf_{x \in \mathcal{F}} \lambda_n \left(J^T(x) J(x) \right)$$

is strictly positive. Consider the function

$$f(x) = \frac{1}{2} \sum_{i=1}^m g_i^2(x).$$

Clearly, $f(x^*) = 0$. Note that $f'(x) = J(x)g(x)$. Therefore

$$\|f'(x)\|^2 = \langle (J^T(x)J(x))g(x), g(x) \rangle \geq \sigma \|g(x)\|^2 = 2\sigma(f(x) - f(x^*)).$$

Thus, f is a gradient dominated function on \mathcal{F} of degree two with $\tau_f = \frac{1}{2\sigma}$. Note that, for $m < n$, the set of solutions to (4.9) is *not* a singleton and therefore the Hessians of function f are necessarily degenerate at the solutions. \square

In order to study the complexity of minimization of the gradient dominated functions we need one more auxiliary result.

Lemma 7 *At each step of method (3.3) we can guarantee the following decrease of the objective function:*

$$f(x_k) - f(x_{k+1}) \geq \frac{L_0 \|f'(x_{k+1})\|^{3/2}}{3\sqrt{2} \cdot (L+L_0)^{3/2}}, \quad k \geq 0. \quad (4.10)$$

Proof:

In view of inequality (2.11) and (2.9) we get

$$f(x_k) - f(x_{k+1}) \geq \frac{M_k}{12} r_{M_k}^3(x_k) \geq \frac{M_k}{12} \left(\frac{2\|f'(x_{k+1})\|}{L+M_k} \right)^{3/2} = \frac{M_k \|f'(x_{k+1})\|^{3/2}}{3\sqrt{2} \cdot (L+M_k)^{3/2}}.$$

It remains to note that the right-hand side of this inequality is increasing in $M_k \leq 2L$. Thus, we can replace M_k by its lower bound L_0 . \square

Let us start from the analysis of the gradient dominated functions of degree one.

Theorem 6 *Let us apply method (3.3) to minimization of a gradient dominated function $f(x)$ of degree $p = 1$.*

1. *If the initial value of the objective function is large enough:*

$$f(x_0) - f(x^*) \geq \hat{\omega} \equiv \frac{18}{L_0^2} \tau_f^3 \cdot (L + L_0)^3,$$

then the process converges to the region $\mathcal{L}(\hat{\omega})$ superlinearly:

$$\ln \left(\frac{1}{\hat{\omega}} (f(x_k) - f(x^*)) \right) \leq \left(\frac{2}{3} \right)^k \ln \left(\frac{1}{\hat{\omega}} (f(x_0) - f(x^*)) \right). \quad (4.11)$$

2. *If $f(x_0) - f(x^*) \leq \gamma^2 \hat{\omega}$ for some $\gamma > 1$, then we have the following estimate for the rate of convergence:*

$$f(x_k) - f(x^*) \leq \hat{\omega} \cdot \frac{\gamma^2 (2 + \frac{3}{2}\gamma)^2}{(2 + (k + \frac{3}{2}) \cdot \gamma)^2}, \quad k \geq 0. \quad (4.12)$$

Proof:

Using inequalities (4.10) and (4.7) with $p = 1$ we get

$$f(x_k) - f(x_{k+1}) \geq \frac{L_0 \cdot (f(x_{k+1}) - f(x^*))^{3/2}}{3\sqrt{2} \cdot (L+L_0)^{3/2} \cdot \tau_f^{3/2}} = \hat{\omega}^{-1/2} (f(x_{k+1}) - f(x^*))^{3/2}.$$

Denoting $\delta_k = (f(x_k) - f(x^*))/\hat{\omega}$, we obtain

$$\delta_k - \delta_{k+1} \geq \delta_{k+1}^{3/2}. \quad (4.13)$$

Hence, as far as $\delta_k \geq 1$, we get

$$\ln \delta_k \leq \left(\frac{2}{3}\right)^k \ln \delta_0,$$

and that is (4.11).

Let us prove now inequality (4.12). Using inequality (4.13), we have

$$\begin{aligned} \frac{1}{\sqrt{\delta_{k+1}}} - \frac{1}{\sqrt{\delta_k}} &\geq \frac{1}{\sqrt{\delta_{k+1}}} - \frac{1}{\sqrt{\delta_{k+1} + \delta_{k+1}^{3/2}}} = \frac{\sqrt{\delta_{k+1} + \delta_{k+1}^{3/2}} - \sqrt{\delta_{k+1}}}{\sqrt{\delta_{k+1}} \sqrt{\delta_{k+1} + \delta_{k+1}^{3/2}}} \\ &= \frac{1}{\sqrt{1 + \sqrt{\delta_{k+1}}} \cdot \left(1 + \sqrt{1 + \sqrt{\delta_{k+1}}}\right)} = \frac{1}{1 + \sqrt{\delta_{k+1}} + \sqrt{1 + \sqrt{\delta_{k+1}}}} \\ &\geq \frac{1}{2 + \frac{3}{2}\sqrt{\delta_{k+1}}} \geq \frac{1}{2 + \frac{3}{2}\sqrt{\delta_0}}. \end{aligned}$$

Thus, $\frac{1}{\delta_k} \geq \frac{1}{\gamma} + \frac{k}{2 + \frac{3}{2}\gamma}$, and this is (4.12). \square

Let us look now at the gradient dominated functions of degree two.

Theorem 7 *Let us apply method (3.3) to minimization of a gradient dominated function $f(x)$ of degree $p = 2$.*

1. *If the initial value of the objective function is large enough:*

$$f(x_0) - f(x^*) \geq \tilde{\omega} \equiv \frac{L_0^4}{324(L+L_0)^6 \tau_f^3}, \quad (4.14)$$

at its first phase the process converges with the following rate:

$$f(x_k) - f(x^*) \leq (f(x_0) - f(x^*)) \cdot e^{-k \cdot \sigma}, \quad (4.15)$$

where $\sigma = \frac{\tilde{\omega}^{1/4}}{\tilde{\omega}^{1/4} + (f(x_0) - f(x^*))^{1/4}}$. *This phase ends on the first iteration k_0 , for which (4.14) does not hold.*

2. *For $k \geq k_0$ the rate of convergence is super-linear:*

$$f(x_{k+1}) - f(x^*) \leq \tilde{\omega} \cdot \left(\frac{f(x_k) - f(x^*)}{\tilde{\omega}}\right)^{4/3}. \quad (4.16)$$

Proof:

Using inequalities (4.10) and (4.7) with $p = 2$ we get

$$f(x_k) - f(x_{k+1}) \geq \frac{L_0 \cdot (f(x_{k+1}) - f(x^*))^{3/4}}{3\sqrt{2} \cdot (L+L_0)^{3/2} \cdot \tau_f^{3/4}} = \tilde{\omega}^{1/4} (f(x_{k+1}) - f(x^*))^{3/4}.$$

Denoting $\delta_k = (f(x_k) - f(x^*)) / \tilde{\omega}$ we obtain

$$\delta_k \geq \delta_{k+1} + \delta_{k+1}^{3/4}. \quad (4.17)$$

Hence,

$$\frac{\delta_k}{\delta_{k+1}} \geq 1 + \delta_k^{-1/4} \geq 1 + \delta_0^{-1/4} = \frac{1}{1-\sigma} \geq e^\sigma,$$

and we get (4.15). Finally, from (4.17) we have $\delta_{k+1} \leq \delta_k^{4/3}$, and that is (4.16). \square

Comparing the statement of Theorem 7 with other theorems of this section we see a significant difference: this is the first time when the initial gap $f(x_0) - f(x^*)$ enters the complexity estimate of the first phase of the process in a polynomial way; in all other cases the dependence on this gap is much weaker.

4.3 Nonlinear transformations of convex functions

Let $u(x) : R^n \rightarrow R^n$ be a non-degenerate operator. Denote by $v(u)$ its inverse:

$$v(u) : R^n \rightarrow R^n, \quad v(u(x)) \equiv x.$$

Consider the following function:

$$f(x) = \phi(u(x)),$$

where $\phi(u)$ is a convex function with bounded level sets. Denote by $x^* \equiv v(u^*)$ its minimum. Let us fix some $x_0 \in R^n$. Denote

$$\sigma = \max_u \{\|v'(u)\| : \phi(u) \leq f(x_0)\},$$

$$D = \max_u \{\|u - u^*\| : \phi(u) \leq f(x_0)\}.$$

The following result is straightforward.

Lemma 8 *For any $x, y \in \mathcal{L}(f(x_0))$ we have*

$$\|x - y\| \leq \sigma \|u(x) - u(y)\|. \quad (4.18)$$

Proof:

Indeed, for $x, y \in \mathcal{L}(f(x_0))$, we have $\phi(u(x)) \leq f(x_0)$ and $\phi(u(y)) \leq f(x_0)$. Consider the trajectory $x(t) = v(tu(y) + (1-t)u(x))$, $t \in [0, 1]$. Then

$$y - x = \int_0^1 x'(t) dt = \left(\int_0^1 v'(tu(y) + (1-t)u(x)) dt \right) \cdot (u(y) - u(x)),$$

and (4.18) follows. \square

The following result is very similar to Theorem 4.

Theorem 8 Assume that function f has Lipschitz continuous Hessian on $\mathcal{F} \supseteq \mathcal{L}(f(x_0))$. And let the sequence $\{x_k\}$ be generated by method (3.3).

1. If $f(x_0) - f^* \geq \frac{3}{2}L(\sigma D)^3$, then $f(x_1) - f^* \leq \frac{1}{2}L(\sigma D)^3$.
2. If $f(x_0) - f^* \leq \frac{3}{2}L(\sigma D)^3$, then the rate of convergence of the process (3.3) is as follows:

$$f(x_k) - f(x^*) \leq \frac{3L(\sigma D)^3}{2(1+\frac{1}{3}k)^2}, \quad k \geq 0. \quad (4.19)$$

Proof:

Indeed, in view of inequality (2.10), upper bound on the parameters M_k and definition (4.1), for any $k \geq 0$ we have:

$$f(x_{k+1}) - f(x^*) \leq \min_y [f(y) - f(x^*) + \frac{L}{2}\|y - x_k\|^3 :$$

$$y = v(\alpha u^* + (1 - \alpha)u(x_k)), \alpha \in [0, 1]].$$

By definition of points y in the above minimization problem and (4.18), we have

$$f(y) - f(x^*) = \phi(\alpha u^* + (1 - \alpha)u(x_k)) - \phi(u^*) \leq (1 - \alpha)(f(x_k) - f(x^*)),$$

$$\|y - x_k\| \leq \alpha \sigma \|u(x_k) - u^*\| \leq \alpha \sigma D.$$

This means that the reasoning of Theorem 4 goes through with replacement D by σD . \square

Let us prove a statement on strongly convex ϕ . Denote $\tilde{\omega} = \frac{1}{L^2} \left(\frac{\gamma}{2\sigma^2} \right)^3$.

Theorem 9 Let function ϕ be strongly convex with convexity parameter $\gamma > 0$. Then, under assumptions of Theorem 8, the performance of the scheme (3.3) is as follows.

1. If $f(x_0) - f(x^*) \geq \frac{4}{9}\tilde{\omega}$, then at the first phase of the process we get the following rate of convergence:

$$f(x_k) - f(x^*) \leq \left[(f(x_0) - f(x^*))^{1/4} - \frac{k}{6} \sqrt{\frac{2}{3}} \tilde{\omega}^{1/4} \right]^4. \quad (4.20)$$

This phase is terminated as soon as $f(x_{k_0}) - f(x^*) \leq \frac{4}{9}\tilde{\omega}$ for some $k_0 \geq 0$.

2. For $k \geq k_0$ the sequence converges superlinearly:

$$f(x_{k+1}) - f(x^*) \leq \frac{1}{2}(f(x_k) - f(x^*)) \sqrt{\frac{f(x_k) - f(x^*)}{\tilde{\omega}}}. \quad (4.21)$$

Proof:

Indeed, in view of inequality (2.10), upper bound on the parameters M_k and definition (4.1), for any $k \geq 0$ we have:

$$f(x_{k+1}) - f(x^*) \leq \min_y [f(y) - f(x^*) + \frac{L}{2}\|y - x_k\|^3 :$$

$$y = v(\alpha u^* + (1 - \alpha)u(x_k)), \alpha \in [0, 1]].$$

By definition of points y in the above minimization problem and (4.18), we have

$$\begin{aligned} f(y) - f(x^*) &= \phi(\alpha u^* + (1 - \alpha)u(x_k)) - \phi(u^*) \leq (1 - \alpha)(f(x_k) - f(x^*)), \\ \|y - x_k\| &\leq \alpha\sigma\|u(x_k) - u^*\| \leq \alpha\sigma\sqrt{\frac{2}{\gamma}(f(x_0) - f(x^*))}. \end{aligned}$$

This means that the reasoning of Theorem 5 goes through with replacement L by $\sigma^3 L$. \square

Note that the functions discussed in this section are often used as test functions for non-convex optimization algorithms.

5 Implementation issues

5.1 Solving the cubic regularization

Note that the auxiliary minimization problem (2.4), which we need to solve in order to compute the mapping $T_M(x)$, namely,

$$\min_{h \in R^n} \left[\langle g, h \rangle + \frac{1}{2} \langle Hh, h \rangle + \frac{M}{6} \|h\|^3 \right], \quad (5.1)$$

is substantially nonconvex. It can have isolated strict local minima, while we need to find a global one. Nevertheless, as we will show in this section, this problem is equivalent to a convex one-dimensional optimization problem.

Before we present an “algorithmic” proof of this fact, let us provide it with a general explanation. Introduce the following objects:

$$\begin{aligned} \xi_1(h) &= \langle g, h \rangle + \frac{1}{2} \langle Hh, h \rangle, \quad \xi_2(h) = \|h\|^2, \\ Q &= \left\{ \xi = (\xi^{(1)}, \xi^{(2)})^T : \xi^{(1)} = \xi_1(h), \xi^{(2)} = \xi_2(h), h \in R^n \right\} \subset R^2, \\ \varphi(\xi) &= \xi^{(1)} + \frac{M}{6} \left(\xi^{(2)} \right)_+^{3/2}. \end{aligned}$$

where $(a)_+ = \max\{a, 0\}$. Then

$$\begin{aligned} \min_{h \in R^n} \left[\langle g, h \rangle + \frac{1}{2} \langle Hh, h \rangle + \frac{M}{6} \|h\|^3 \right] &\equiv \min_{h \in R^n} \left[\xi_1(h) + \frac{M}{6} \xi_2^{3/2}(h) \right] \\ &= \min_{\xi \in Q} \varphi(\xi). \end{aligned}$$

Theorem 2.2 in [14] guarantees that for $n \geq 2$ the set Q is *convex and closed*. Thus we have reduced the initial nonconvex minimization problem in R^n to a convex unconstrained minimization problem in R^2 . Up to this moment, this reduction is not constructive, because Q is given in implicit form. However, the next statement shows that the description of this set is quite simple.

Denote

$$v_u(h) = \langle g, h \rangle + \frac{1}{2} \langle Hh, h \rangle + \frac{M}{6} \|h\|^3, \quad h \in R^n,$$

and

$$v_l(r) = -\frac{1}{2}\langle (H + \frac{Mr}{2}I)^{-1}g, g \rangle - \frac{M}{12}r^3.$$

For the first function sometimes we use the notation $v_u(g; h)$. Denote

$$\mathcal{D} = \{r \in \mathbb{R} : H + \frac{Mr}{2}I \succ 0, r \geq 0\}.$$

Theorem 10 *For any $M > 0$ we have the following relation:*

$$\min_{h \in \mathbb{R}^n} v_u(h) = \sup_{r \in \mathcal{D}} v_l(r). \quad (5.2)$$

For any $r \in \mathcal{D}$, direction $h(r) = -\left(H + \frac{Mr}{2}I\right)^{-1}g$ satisfies equation

$$0 \leq v_u(h(r)) - v_l(r) = \frac{M}{12}(r + 2\|h(r)\|)(\|h(r)\| - r)^2 = \frac{4}{3M} \cdot \frac{r+2\|h(r)\|}{(r+\|h(r)\|)^2} \cdot v_l'(r)^2. \quad (5.3)$$

Proof:

Denote the left-hand side of relation (5.2) by v_u^* , and its right-hand side by v_l^* . Let us show that $v_u^* \geq v_l^*$. Indeed,

$$\begin{aligned} v_u^* &= \min_{h \in \mathbb{R}^n} \left[\langle g, h \rangle + \frac{1}{2}\langle Hh, h \rangle + \frac{M}{6}\|h\|^3 \right] \\ &= \min_{\substack{h \in \mathbb{R}^n, \\ \tau = \|h\|^2}} \left[\langle g, h \rangle + \frac{1}{2}\langle Hh, h \rangle + \frac{M}{6}(\tau)_+^{3/2} \right] \\ &= \min_{\substack{h \in \mathbb{R}^n, \\ \tau \in \mathbb{R}}} \sup_{r \in \mathbb{R}} \left[\langle g, h \rangle + \frac{1}{2}\langle Hh, h \rangle + \frac{M}{6}(\tau)_+^{3/2} + \frac{M}{4}r(\|h\|^2 - \tau) \right] \\ &\geq \sup_{r \in \mathcal{D}} \min_{\substack{h \in \mathbb{R}^n, \\ \tau \in \mathbb{R}}} \left[\langle g, h \rangle + \frac{1}{2}\langle Hh, h \rangle + \frac{M}{6}(\tau)_+^{3/2} + \frac{M}{4}r(\|h\|^2 - \tau) \right] \equiv v_l^*. \end{aligned}$$

Consider now an arbitrary $r \in \mathcal{D}$. Then

$$g = -Hh(r) - \frac{M}{2}rh(r).$$

Therefore

$$\begin{aligned} v_u(h(r)) &= \langle g, h(r) \rangle + \frac{1}{2}\langle Hh(r), h(r) \rangle + \frac{M}{6}\|h(r)\|^3 \\ &= -\frac{1}{2}\langle Hh(r), h(r) \rangle - \frac{M}{2}r\|h(r)\|^2 + \frac{M}{6}\|h(r)\|^3 \\ &= -\frac{1}{2}\langle (H + \frac{Mr}{2}I)h(r), h(r) \rangle - \frac{M}{4}r\|h(r)\|^2 + \frac{M}{6}\|h(r)\|^3 \\ &= v_l(r) + \frac{M}{12}r^3 - \frac{M}{4}r\|h(r)\|^2 + \frac{M}{6}\|h(r)\|^3 \\ &= v_l(r) + \frac{M}{12}(r + 2\|h(r)\|) \cdot (\|h(r)\| - r)^2. \end{aligned}$$

Thus, relation (5.3) is proved.

Note that

$$v'_l(r) = \frac{M}{4}(\|h(r)\|^2 - r^2).$$

Therefore, if the optimal value v_l^* is attained at some $r^* > 0$ from \mathcal{D} , then $v'_l(r^*) = 0$ and by (5.3) we conclude that $v_r^* = v_l^*$. If $r^* = \frac{2}{M}(-\lambda_n(H))_+$, then equality (5.2) can be justified by continuity arguments (since $v_u^* \equiv v_u^*(g)$ is a concave function in $g \in R^n$; see also the discussion below). \square

Note that Proposition 1 follows from the definition of set \mathcal{D} .

Theorem 10 demonstrates that in the non-degenerate situation the solution of the problem (5.2) can be found from the one-dimensional equation

$$r = \left\| \left(H + \frac{Mr}{2}I \right)^{-1} g \right\|, \quad r \geq \frac{2}{M}(-\lambda_n(H))_+. \quad (5.4)$$

A technique for solving such equations is very well developed for the needs of trust region methods (see [2], Chapter 7, for exhaustive expositions of the different approaches). As compared with (5.4), the equation arising in trust region schemes has a constant left-hand side. But of course, all possible difficulties in this equation are due to the non-linear (convex) right-hand side.

For completeness of presentation, let us briefly discuss the structure of equation (5.4). In the basis of eigenvectors of matrix H this equation can be written as

$$r^2 = \sum_{i=1}^n \frac{\tilde{g}_i^2}{(\lambda_i + \frac{Mr}{2})^2}, \quad r \geq \frac{2}{M}(-\lambda_n)_+, \quad (5.5)$$

where λ_i are eigenvalues of matrix H and \tilde{g}_i are coordinates of vector g in the new basis.

If $\tilde{g}_n \neq 0$, then the solution r^* of equation (5.5) is in the interior of the domain:

$$r > \frac{2}{M}(-\lambda_n)_+,$$

and we can compute the displacement $h(r^*)$ by the explicit expression:

$$h(g; r^*) = - \left(H + \frac{Mr^*}{2}I \right)^{-1} g.$$

If $\tilde{g}_n = 0$ then this formula does not work and we have to consider different cases. In order to avoid all these complications, let us mention the following simple result.

Lemma 9 *Let $g_n = 0$. Define $g(\epsilon) = \tilde{g} + \epsilon e_n$, where e_n is the n th coordinate orth. Denote by $r^*(\epsilon)$ the solution of equation (5.5) with $\tilde{g} = g(\epsilon)$. Then any limit point of the trajectory*

$$h(g(\epsilon); r^*(\epsilon)), \quad \epsilon \rightarrow 0,$$

is a global minimum in h of function $v_u(g; h)$.

Proof:

Indeed, function $v_u^*(g)$ is concave for $g \in R^n$. Therefore it is continuous. Hence,

$$v_u^*(g) = \lim_{\epsilon \rightarrow 0} v_u^*(g(\epsilon)) = \lim_{\epsilon \rightarrow 0} v_u(g(\epsilon); h(g(\epsilon); r^*(\epsilon))).$$

It remains to note that the function $v_u(g; h)$ is continuous in both arguments. \square

In order to illustrate the difficulties arising in the dual problem, let us look at an example.

Example 4 Let $n = 2$ and

$$\tilde{g} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad \lambda_1 = 0, \quad \lambda_2 = -1, \quad M = 1.$$

Thus, our primal problem is as follows:

$$\min_{h \in \mathbb{R}^2} \left\{ \psi(h) \equiv -h^{(1)} - \frac{1}{2} \left(h^{(2)} \right)^2 + \frac{1}{6} \left[\sqrt{\left(h^{(1)} \right)^2 + \left(h^{(2)} \right)^2} \right]^3 \right\}.$$

Following to (2.5), we have to solve the following system of non-linear equations:

$$\begin{aligned} \frac{h^{(1)}}{2} \sqrt{\left(h^{(1)} \right)^2 + \left(h^{(2)} \right)^2} &= 1, \\ \frac{h^{(2)}}{2} \sqrt{\left(h^{(1)} \right)^2 + \left(h^{(2)} \right)^2} &= h^{(2)}. \end{aligned}$$

Thus, we have three candidate solutions:¹

$$h_1^* = \begin{pmatrix} \sqrt{2} \\ 0 \end{pmatrix}, \quad h_2^* = \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad h_3^* = \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix}.$$

By direct substitution we can see that

$$\psi(h_1^*) = -\frac{2\sqrt{2}}{3} > -\frac{7}{6} = \psi(h_2^*) = \psi(h_3^*).$$

Thus, both h_2^* and h_3^* are our global solutions.

Let us look at the dual problem:

$$\sup_r \left[\phi(r) \equiv -\frac{r^3}{12} - \frac{1}{2} \cdot \frac{1}{0 + \frac{1}{2}r} = -\frac{r^3}{12} - \frac{1}{r} : -1 + \frac{1}{2}r > 0 \right].$$

Note that $\phi'(r) = -\frac{r^2}{4} + \frac{1}{r^2}$. Thus, $\phi'(2) = -\frac{3}{4} < 0$ and we conclude that

$$r^* = 2, \quad \phi^* = -\frac{7}{6}.$$

However, r^* does not satisfy the equation $\phi'(r) = 0$ and the object $h(r^*)$ is not defined.
□

Let us conclude this section with a precise description of the solution of primal problem in (5.2) in terms of the eigenvalues of matrix H . Denote by $\{s_i\}_{i=1}^n$ an orthonormal basis of eigenvectors of H , and let \hat{k} satisfy the conditions

$$\begin{aligned} \tilde{g}^{(i)} &\neq 0 \quad \text{for } i < \hat{k}, \\ \tilde{g}^{(i)} &= 0 \quad \text{for } i \geq \hat{k}. \end{aligned}$$

¹This example demonstrates the reason why the equation (2.5) can have up to $2n$ candidate solutions.

Assume that r^* is the solution to the dual problem in (5.2). Then the solution of the primal problem is given by the vector

$$h^* = - \sum_{i=1}^{\hat{k}-1} \frac{\tilde{g}^{(i)} s_i}{\lambda_i + \frac{M}{2} r^*} + \sigma s_n,$$

where σ is chosen in accordance to the condition $\|h^*\| = r^*$. Note that this rule works also for $\hat{k} = 1$ or $\hat{k} = n + 1$.

We leave justification of above rule as an exercise for the reader. As far as we know, a technique for finding h^* without computation of the basis of eigenvalues is not known yet.

5.2 Line search strategies

Let us discuss the possible computational cost of Step 1 in the method (3.3), which consists of finding $M_k \in [L_0, 2L]$ satisfying the equation:

$$f(T_{M_k}(x)) \leq \bar{f}_{M_k}(x_k).$$

Note that for $M_k \geq L$ this inequality holds. Consider now the strategy

$$\mathbf{while} \ f(T_{M_k}(x)) > f(x_k) \ \mathbf{do} \ M_k := 2M_k; \quad M_{k+1} := M_k. \quad (5.6)$$

It is clear that if we start the process (3.3) with any $M_0 \in [L_0, 2L]$, then the above procedure, as applied at each iteration of the method, has the following advantages:

- $M_k \leq 2L$.
- The total amount of additional computations of the mappings $T_{M_k}(x)$ during the whole process (3.3) is bounded by

$$\log_2 \frac{2L}{L_0}.$$

This amount does not depend on the number of iterations in the main process.

However, it may be that the rule (5.6) is too conservative. Indeed, we can only increase our estimate for the constant L and never come back. This may force the method to take only the short steps. A more reasonable strategy looks as follows:

$$\begin{aligned} \mathbf{while} \ f(T_{M_k}(x)) > f(x_k) \ \mathbf{do} \ M_k := 2M_k; \\ x_{k+1} := T_{M_k}(x_k); \quad M_{k+1} := \max\{\frac{1}{2}M_k, L_0\}. \end{aligned} \quad (5.7)$$

Then it is easy to prove by induction that N_k , the total number of computations of mappings $T_M(x)$ made by (5.7) during the first k iterations, is bounded as follows:

$$N_k \leq 2k + \log_2 \frac{M_k}{L_0}.$$

Thus, if N is the number of iterations in this process, then we compute at most

$$2N + \log_2 \frac{2L}{L_0}$$

mappings $T_M(x)$. That seems to be a reasonable price to pay for the possibility to go by long steps.

6 Discussion

Let us compare the results presented in this paper with some known facts on global efficiency of other minimization schemes. Since there is almost no such results for non-convex case, let us look at some simple class of convex problems.

Assume that function $f(x)$ is strongly convex on R^n with convexity parameter $\gamma > 0$ (see (4.8)). In this case there exists its unique minimum x^* and condition (4.3) holds for all $x \in R^n$ (see, for example, [10], Section 2.1.3). Assume also that Hessian of $f(x)$ is Lipschitz continuous:

$$\|f''(x) - f''(y)\| \leq L\|x - y\|, \quad \forall x, y \in R^n.$$

For such functions, let us obtain the complexity bounds of method (3.3) using the results of Theorems 4 and 5.

Let us fix some $x_0 \in R^n$. Denote by D the *radius* of its level set:

$$D = \max_x \{\|x - x^*\| : f(x) \leq f(x_0)\}.$$

From (4.3) we get

$$D \leq \left[\frac{2}{\gamma} (f(x_0) - f(x^*)) \right]^{1/2}.$$

We will see that it is natural to measure the quality of starting point x_0 by the following characteristic:

$$\kappa \equiv \kappa(x_0) = \frac{LD}{\gamma}.$$

Let us introduce three switching values

$$\omega_0 = \frac{\gamma^3}{18L^2} \equiv \frac{4}{9}\bar{\omega}, \quad \omega_1 = \frac{3}{2}\gamma D^2, \quad \omega_2 = \frac{3}{2}LD^3.$$

In view of Theorem 4, we can reach the level $f(x_0) - f(x^*) \leq \frac{1}{2}LD^3$ in one additional iteration. Therefore without loss of generality we assume that

$$f(x_1) - f(x^*) \leq \omega_2.$$

Assume also that we are interested in a very high accuracy of the solution. Note that the case $\kappa \leq 1$ is very easy since the first iteration of method (3.3) comes very close to the region of super-linear convergence (see Item 2 of Theorem 5).

Consider the case $\kappa \geq 1$. Then $\omega_0 \leq \omega_1 \leq \omega_2$. Let us estimate the duration of the following phases:

$$\text{Phase 1: } \omega_1 \leq f(x_i) \leq \omega_2,$$

$$\text{Phase 2: } \omega_0 \leq f(x_i) \leq \omega_1,$$

$$\text{Phase 3: } \epsilon \leq f(x_i) \leq \omega_0.$$

In view of Theorem 4, the duration of the first phase is bounded as follows:

$$\omega_1 \leq \frac{3LD^3}{2(1+\frac{1}{3}k_1)^2}.$$

Thus, $k_1 \leq 3\sqrt{\kappa}$. Further, in view of Item 1 of Theorem 5, we can bound the duration of the second phase:

$$\omega_0^{1/4} \leq (f(x_{k_1+1}) - f(x^*))^{1/4} - \frac{k_2}{6}\omega_0^{1/4} \leq (\frac{1}{2}\gamma D^2)^{1/4} - \frac{k_2}{6}\omega_0^{1/4}.$$

This gives the following bound: $k_2 \leq 3^{3/4} 2^{1/2} \sqrt{\kappa} \leq 3.25\sqrt{\kappa}$.

Finally, denote $\delta_k = \frac{1}{4\omega_0}(f(x_k) - f(x^*))$. In view of inequality (4.5) we have:

$$\delta_{k+1} \leq \delta_k^{3/2}, \quad k \geq \bar{k} \equiv k_1 + k_2 + 1.$$

At the same time $f(x_{\bar{k}}) - f(x^*) \leq \omega_0$. Thus, $\delta_{\bar{k}} \leq \frac{1}{4}$ and the bound on the duration of the last phase can be found from inequality

$$4\left(\frac{3}{2}\right)^{k_3} \leq \frac{4\omega_0}{\epsilon}.$$

Thus, $k_3 \leq \log_{\frac{3}{2}} \log_4 \frac{2\gamma^3}{9\epsilon L^2}$. Putting all bounds together, we obtain that the total number of steps N in (3.3) is bounded as follows:

$$N \leq 6.25\sqrt{\frac{LD}{\gamma}} + \log_{\frac{3}{2}} \left(\log_4 \frac{1}{\epsilon} + \log_4 \frac{2\gamma^3}{9L^2} \right). \quad (6.1)$$

It is interesting that in estimate (6.1) the parameters of our problem interact with accuracy in an *additive* way. Recall that usually such an interaction is multiplicative. Let us estimate, for example, the complexity of our problem for an optimal method for strongly convex functions with Lipschitz continuous gradient (see [10], Section 2.2.1). Denote by \hat{L} the largest eigenvalue of matrix $f''(x^*)$. Then can guarantee that

$$\gamma I \leq f''(x) \leq (\hat{L} + LD)I \quad \forall x, \|x - x^*\| \leq D.$$

Thus, the complexity bound for the optimal method is of the order

$$O\left(\sqrt{\frac{\hat{L}+LD}{\gamma}} \ln \frac{(\hat{L}+LD)D^2}{\epsilon}\right)$$

iterations. For gradient method it is much worse:

$$O\left(\frac{\hat{L}+LD}{\gamma} \ln \frac{(\hat{L}+LD)D^2}{\epsilon}\right).$$

Thus, we conclude that the global complexity estimates of the modified Newton scheme (3.3) are incomparably better than the estimates of the gradient schemes. At the same time, we should remember, of course, about the difference in the computational cost of each iteration.

Note that the similar bounds can be obtained for other classes of non-convex problems. For example, for nonlinear transformations of convex functions (see Section 4.3), the complexity bound is as follows:

$$N \leq 6.25\sqrt{\frac{\sigma}{\gamma}LD} + \log_{\frac{3}{2}} \left(\log_4 \frac{1}{\epsilon} + \log_4 \frac{2\gamma^3}{9\sigma^6 L^2} \right). \quad (6.2)$$

To conclude, note that in the scheme (3.3) it is possible to find elements of Levenberg-Marquardt approach (see relation (2.7)), or a trust-region approach (see Theorem 10 and related discussion), or a line-search technique (see the rule of Step 1 in (3.3)). However, all these facts are *consequences* of the main idea of the scheme, that is the choice of the next test point as a global minimizer of an upper second-order approximation of the objective function.

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