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Methods: Attraction, Repulsion
and Selection**

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ON CONVERGENCE OF MINIMIZATION METHODS: ATTRACTION, REPULSION AND SELECTION*

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Abstract.

In this paper, we introduce a rather straightforward but fundamental observation concerning the convergence of the general iteration process

$$x^{k+1} = x^k - \alpha(x^k)B(x^k)^{-1}\nabla f(x^k)$$

for minimizing a function $f(x)$. We give necessary and sufficient conditions for a stationary point of $f(x)$ to be a point of strong attraction of the iteration process. We will discuss various ramifications of this fundamental result, particularly for nonlinear least squares problems.

Key words. Strong attraction, weak repulsion, selective minimization.

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1. Introduction. We consider the unconstrained minimization problem

$$(1.1) \quad \min f(x),$$

where $f : \mathfrak{X}^n \rightarrow \mathfrak{R}$ is assumed to be twice (Frechet) differentiable, and the general iteration:

$$(1.2) \quad x^{k+1} = x^k - \alpha^k(B^k)^{-1}\nabla f(x^k).$$

This iterative framework has been studied extensively and many results are available for various choices of α^k and B^k that guarantee convergence, see the classic books by Ortega and Rheinboldt [6], and Dennis and Schnabel [2] on this subject.

A less frequently asked question is the following. Given certain conditions on α^k and B^k , what type of stationary points of $f(x)$ are or are not points of attraction of the iteration (1.2)? In this paper, we try to shed some light on this question.

The spectral radius of a matrix M will be denoted by $\rho(M)$, and an eigenvalue by $\lambda_i(M)$. Moreover, $\lambda_{\max}(M)$ and $\lambda_{\min}(M)$ are the maximum and minimum eigenvalues of a symmetric matrix M . We use the usual partial ordering for symmetric matrices: $A \succeq B$ means $A - B$ is positive semidefinite; similarly for other relationships \preceq , \succ and \prec . The norm $\|\cdot\|$ will be either the Euclidean norm for vectors or the norm it induces for matrices, unless otherwise specified.

2. Iterative Methods. Most iterative methods can be represented as a fixed-point iteration:

$$(2.1) \quad x^{k+1} = T(x^k)$$

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for some function $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$. For unconstrained minimization, $T(x)$ is often defined through (1.2), namely,

$$(2.2) \quad T(x) = x - \alpha(x)B(x)^{-1}\nabla f(x).$$

This iterative framework includes Newton's method, quasi-Newton methods and gradient methods with variant step-length control schemes. In the case of nonlinear least squares problems, it also includes the Gauss-Newton and the Levenberg-Marquardt methods.

It is clear that any stationary point of $f(x)$ is a fixed point of the iteration (2.1). In order to classify fixed points of (2.1), we will need the derivative of $T(x)$, $T'(x)$, at stationary points of $f(x)$. The following proposition shows that for $T'(x)$ to exist at a stationary point x^* of $f(x)$, the function $\alpha(x)B(x)^{-1}$ need not be differentiable at x^* ; instead, continuity at x^* will suffice. This result is a special case of **10.2.1** in Ortega and Rheinboldt [6]. For completeness, we include a short proof.

PROPOSITION 2.1. *Let x^* be a stationary point of $f(x)$. Assume that $\alpha(x)$ and $B(x)$ are continuous at x^* where $B(x)$ is also nonsingular. Then the derivative of $T(x)$ in (2.2) exists at x^* , and*

$$(2.3) \quad T'(x^*) = I - \alpha(x^*)B(x^*)^{-1}\nabla^2 f(x^*).$$

Proof. Let $H(x) \equiv \alpha(x)B(x)^{-1}$. It suffices to show that the derivative of $H(x)\nabla f(x)$ exists at x^* and is $H(x)\nabla^2 f(x)$. The continuity of $\alpha(x)$ and $B(x)$ at x^* plus the nonsingularity of $B(x^*)$ imply the continuity of $H(x)$ at x^* . Noting $\nabla f(x^*) = 0$, we consider

$$\begin{aligned} & [H(x^* + h)\nabla f(x^* + h) - H(x^*)\nabla f(x^*) - H(x^*)\nabla^2 f(x^*)h]/\|h\| \\ &= H(x^* + h)[\nabla f(x^* + h) - \nabla f(x^*) - \nabla^2 f(x^*)h]/\|h\| \\ & \quad + [H(x^* + h) - H(x^*)](\nabla^2 f(x^*)h/\|h\|). \end{aligned}$$

By continuity of $H(x)$ and differentiability of $f(x)$ at x^* , both terms on the right-hand side vanish as $\|h\| \rightarrow 0$. This completes the proof. \square

3. Points of Attraction and Repulsion. We now give the definition of “point of attraction” of the iteration (2.1), first introduced by Ostrowski (see **10.1.1** in [6] and the references therein).

DEFINITION 3.1 (Attraction). *A fixed point x^* of $T(x)$ is said to be a point of attraction of the iteration (2.1) if there is an open neighborhood N of x^* such that for any point $x^0 \in N$, the iterates $\{x^k\}$ generated by (2.1) all lie in N and converge to x^* .*

The well-known Ostrowski Theorem (**10.1.3** in Ortega and Rheinboldt [6]) says that a sufficient (but not necessary) condition for a stationary point x^* to be a point of attraction of the iteration (2.1) is that the spectral radius of $T'(x^*)$ be less than one, i.e., $\rho(T'(x^*)) < 1$. We call a stationary point satisfying this condition a point of strong attraction.

DEFINITION 3.2 (Strong Attraction). *A fixed point x^* of $T(x)$ is said to be a point of strong attraction of the iteration (2.1) if $T(x)$ is differentiable at x^* and*

$$\rho(T'(x^*)) < 1.$$

Given the iteration (2.1) and certain conditions on the choices of $\alpha(x)$ and $B(x)$, we are interested in knowing what types of stationary points are not or not likely to be points of attraction. To this end, we introduce the following definition.

DEFINITION 3.3 (Weak and Strong Repulsion). *A fixed point x^* of $T(x)$ is said to be a point of weak repulsion of the iteration (2.1) if $T(x)$ is differentiable at x^* and $\rho(T'(x^*)) > 1$, i.e.,*

$$\max_{1 \leq i \leq n} |\lambda_i(T'(x^*))| > 1.$$

Moreover, we say that x^ is a point of strong repulsion of the iteration (2.1) if*

$$\min_{1 \leq i \leq n} |\lambda_i(T'(x^*))| > 1.$$

4. Convergence and Weak Repulsion. In this section, we discuss necessary conditions for a sequence $\{x^k\}$ generated by the iteration (2.1) to converge to a point of weak repulsion. The discussion is for general fixed-point iterations, not necessarily limited to the particular form of (2.2).

At any point of weak repulsion x^* , the iteration (2.1) repels points away from x^* in the eigenvector directions associated with the eigenvalues of $T'(x^*)$ of magnitude greater than one. This fact is given in the following proposition.

PROPOSITION 4.1. *Let x^* be a point of weak repulsion of the iteration (2.1). Then there exists $\bar{\epsilon} > 0$ such that for any $\epsilon \in (0, \bar{\epsilon})$, one can find a point x that satisfies $\|x - x^*\| = \epsilon$ and*

$$\|T(x) - x^*\| > \|x - x^*\|.$$

Proof. Being a point of weak repulsion, $T'(x^*)$ has at least one eigenvalue λ_j satisfying for some $\sigma > 0$

$$|\lambda_j| = 1 + \sigma.$$

It follows from the differentiability of $T(x)$ at x^* that there exists $\bar{\epsilon} > 0$ such that

$$\|T(x) - T(x^*) - T'(x^*)(x - x^*)\| < \sigma \|x - x^*\|,$$

whenever $\|x - x^*\| \leq \bar{\epsilon}$. Given any $\epsilon \in (0, \bar{\epsilon})$, let $x = x^* + \epsilon v$ where v is a unit eigenvector corresponding to λ_j . Hence, we have $\|x - x^*\| = \epsilon$, $T'(x^*)(x - x^*) = \lambda_j(x - x^*)$, and

$$\begin{aligned} \|T(x) - x^*\| &\geq \|T'(x^*)(x - x^*)\| - \|T(x) - T(x^*) - T'(x^*)(x - x^*)\| \\ &> (1 + \sigma)\|x - x^*\| - \sigma\|x - x^*\| \\ &= \|x - x^*\|. \end{aligned}$$

This completes the proof. \square

This proposition implies that the iterates generated by (2.1) cannot approach a point of weak repulsion x^* from the eigenspace associated with an eigenvalue of magnitude greater than one.

Let x^* be a point of weak repulsion of the iteration (2.1) that is not also a point of strong repulsion, i.e.,

$$(4.1) \quad \min_{1 \leq i \leq n} |\lambda_i(T'(x^*))| \leq 1 < \max_{1 \leq i \leq n} |\lambda_i(T'(x^*))|.$$

Suppose that $T'(x^*)$ is diagonalized by a matrix U so that

$$(4.2) \quad U^{-1}T'(x^*)U = \Lambda \equiv \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix},$$

where, without loss of generality, for some $m < n$

$$(4.3) \quad |\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_m| > 1 \geq |\lambda_{m+1}| \geq \cdots \geq |\lambda_n|.$$

Obviously, the columns $\{u_j\}$ of U are eigenvectors of $T'(x^*)$. Moreover, let

$$\sigma \equiv |\lambda_m| - 1 > 0.$$

Then

$$(4.4) \quad |\lambda_j| \geq (1 + \sigma), \quad \forall j \leq m.$$

The following lemma gives necessary conditions for a sequence generated by the iteration (2.1) to converge to a point of weak repulsion.

LEMMA 4.2. *Let x^* be a point of weak repulsion of the iteration (2.1), where $T'(x^*)$ satisfies (4.1) and, together with a nonsingular matrix U , (4.2) and (4.3). If a sequence $\{x^k\}$ generated by (2.1) converges to x^* , then necessarily*

$$(4.5) \quad \lim_{k \rightarrow \infty} \frac{|(U^{-1}(x^k - x^*))_i|}{\|U^{-1}(x^k - x^*)\|} = 0, \quad i = 1, 2, \dots, m.$$

Proof. For a sequence $\{x^k\}$, we define $\{e^k\}$ and $\{d^k\}$ by

$$(4.6) \quad e^k \equiv x^k - x^* \equiv U d^k.$$

In this notation, (4.5) is equivalent to $|(d^k)_i|/\|d^k\| \rightarrow 0$, $i = 1, 2, \dots, m$.

Suppose that (4.5) does not hold for some j , $1 \leq j \leq m$. Then there must exist $k_0 > 1$ and $\tau > 0$ such that $|(d^k)_j|/\|d^k\| > \tau$ for all $k > k_0$, or

$$(4.7) \quad \frac{\|d^k\|}{|(d^k)_j|} < \frac{1}{\tau}, \quad \forall k \geq k_0.$$

Let

$$r^k = T(x^k) - T(x^*) - T'(x^*)(x^k - x^*).$$

By (4.6) and (4.2), we can write the equality

$$x^{k+1} - x^* = T'(x^*)(x^k - x^*) + (T(x^k) - T(x^*) - T'(x^*)(x^k - x^*))$$

into

$$(4.8) \quad U d^{k+1} = T'(x^*)U d^k + r^k = U \Lambda d^k + r^k = U(\Lambda d^k + h^k)$$

where $h^k = U^{-1}r^k$. The equality (4.8) leads to the recursion

$$(4.9) \quad d^{k+1} = \Lambda d^k + h^k.$$

From the definition of r^k , there holds the property: $\|r^k\|/\|e^k\| \rightarrow 0$. Since this property is norm-independent, we have

$$\frac{\|U^{-1}r^k\|}{\|U^{-1}e^k\|} \equiv \frac{\|h^k\|}{\|d^k\|} \rightarrow 0.$$

Hence, there exists $k_1 > 0$ such that for $i = 1, 2, \dots, n$

$$(4.10) \quad \frac{|(h^k)_i|}{\|d^k\|} < \sigma\tau, \quad \forall k > k_1.$$

It follows from (4.9), (4.4), (4.7) and (4.10) that for $k > \max(k_0, k_1)$

$$\begin{aligned} |(d^{k+1})_j| &= |\lambda_j(d^k)_j + (h^k)_j| \\ &\geq (1 + \sigma)|(d^k)_j| - |(h^k)_j| \\ &= |(d^k)_j| + \left(\sigma - \frac{\|d^k\|}{|(d^k)_j|} \frac{|(h^k)_j|}{\|d^k\|} \right) |(d^k)_j| \\ &> |(d^k)_j| + \left(\sigma - \frac{1}{\tau} \sigma\tau \right) |(d^k)_j| \\ &= |(d^k)_j|, \end{aligned}$$

that is,

$$|(d^{k+1})_j| > |(d^k)_j|, \quad \forall k > \max(k_0, k_1).$$

This means that the sequence $\{d^k\}$ does not converge to zero; therefore, neither does $\{e^k\}$ since $e^k = U d^k$ and U is nonsingular. We have proved that if (4.5) does not hold, then $\{x^k\}$ does not converge to x^* . \square

REMARK 4.1. For $T(x)$ defined by (2.2) (therefore $T'(x^*)$ defined by (2.3)), if $B(x^*)$ is symmetric positive definite, then

$$T'(x^*) = B(x^*)^{-1/2} [I - \alpha(x^*) B(x^*)^{-1/2} \nabla^2 f(x^*) B(x^*)^{-1/2}] B(x^*)^{1/2}.$$

Hence, $T'(x^*)$ is similar to a symmetric matrix which is diagonalizable by a real matrix. This, in turn, implies that $T'(x^*)$ itself is diagonalizable by a real matrix. Consequently, Lemma 4.2 holds for such $T(x)$.

The following corollary provides an interpretation of Lemma 4.2.

COROLLARY 4.3. Let $\{e^k\}$ and $\{d^k\}$ be defined as in (4.6), and

$$p^k = (d_1^k, d_2^k, \dots, d_m^k)^T \quad \text{and} \quad q^k = (d_{m+1}^k, d_{m+2}^k, \dots, d_n^k)^T,$$

where m is also in (4.3). Under the assumptions of Lemma 4.2, if a sequence $\{x^k\}$ generated by (2.1) converges to x^* , then necessarily

$$(4.11) \quad \lim_{k \rightarrow \infty} \frac{\|p^k\|}{\|q^k\|} = 0.$$

Proof. By Lemma 4.2, $|(d^k)_i|/\|d^k\| \rightarrow 0$, $i = 1, 2, \dots, m$. Therefore,

$$\frac{\|p^k\|^2}{\|d^k\|^2} = \frac{\|p^k\|^2}{\|p^k\|^2 + \|q^k\|^2} = \frac{1}{1 + (\|q^k\|/\|p^k\|)^2} \rightarrow 0.$$

Consequently, $\|q^k\|/\|p^k\| \rightarrow \infty$, which implies (4.11). \square

Under the assumptions of Lemma 4.2, in order for $\{x^k\}$ to converge to a point of weak repulsion x^* , one must have $p^k = o(\|q^k\|)$; namely, the error components in the eigenspace associated with the eigenvalues of magnitude greater than one must go to zero faster than the rest of the components do. In other words, convergence to x^* can take place, if at all, only asymptotically along the eigenspace associated with the eigenvalues of magnitude not greater than one. Since all proper subspaces of \mathbb{R}^n have zero measure, from a probabilistic viewpoint one may argue that in general convergence to a point of weak repulsion is improbable.

In Section 8, we will report numerical results on the behavior of iterates generated the iteration (2.1)-(2.2) around points of weak repulsion.

To close this section, we mention that it is easy to verify that any sequence $\{x^k\}$ generated by (2.1) cannot converge to a point of strong repulsion x^* , unless $x^k = x^*$ at some finite iteration k .

5. Main Result. We now give our main result of the paper concerning necessary and sufficient conditions for a stationary point to be a point of strong attraction. The result is a rather straightforward observation with many interesting consequences. To the best of our knowledge, this result does not appear in the literature.

THEOREM 5.1. *Let x^* be a stationary point of $f(x)$ and $T(x)$ be defined by (2.2). Assume that*

- (i) $B(x)$ and $\alpha(x)$ are continuous at x^* ,
- (ii) $B(x^*)$ is symmetric positive definite, and $\alpha(x^*) > 0$.

Then

$$\rho(T'(x^*)) \leq 1$$

if and only if

$$(5.1) \quad 0 \preceq \nabla^2 f(x^*) \preceq \frac{2B(x^*)}{\alpha(x^*)}.$$

Moreover, $\rho(T'(x^)) < 1$ if and only if strict inequalities hold in (5.1).*

Proof. We note that $T'(x^*)$ is similar to the symmetric matrix

$$M = I - \alpha(x^*)B(x^*)^{-1/2}\nabla^2 f(x^*)B(x^*)^{-1/2},$$

and $\rho(T'(x^*)) \leq 1$ is equivalent to $-1 \leq \lambda_i(M) \leq 1$, i.e.,

$$-I \preceq M \preceq I.$$

The inequality $M \preceq I$ is equivalent to

$$\alpha(x^*)B(x^*)^{-1/2}\nabla^2 f(x^*)B(x^*)^{-1/2} \succeq 0,$$

which is in turn equivalent to the left inequality of (5.1). On the other hand, the inequality $-I \preceq M$ is equivalent to

$$2I - \alpha(x^*)B(x^*)^{-1/2}\nabla^2 f(x^*)B(x^*)^{-1/2} \succeq 0,$$

or

$$B(x^*)^{-1/2}[2B(x^*) - \alpha(x^*)\nabla^2 f(x^*)]B(x^*)^{-1/2} \succeq 0,$$

which is in turn equivalent to the right inequality of (5.1). This proves (5.1).

The proof of the second assertion is entirely parallel. \square

The left inequality in (5.1) immediately implies the following interesting fact.

COROLLARY 5.2. *Under the assumptions of Theorem 5.1, any stationary point of $f(x)$ where the Hessian matrix has a negative eigenvalue is a point of weak repulsion of the iteration (2.1).*

We recall that a stationary point of $f(x)$ is called a nondegenerate saddle point if the Hessian matrix at this point has both positive and negative eigenvalues. We also recall that a necessary condition for a stationary point of $f(x)$ to be a maximizer is that the Hessian matrix at this point be negative semidefinite. In view of Corollary 5.2, we have the following observation.

REMARK 5.1. *In the iteration (2.1), if one keeps B^k positive definite, then under mild conditions all nondegenerate saddle points of $f(x)$ and all maximizers of $f(x)$ where the Hessian is not the zero matrix are points of weak repulsion; hence, none of these points can be a point of strong attraction of the iteration (2.1).*

We call a stationary point x^* a *strong minimizer* of $f(x)$ if $\nabla^2 f(x^*) \succ 0$. Thus, the left inequality in (5.1) always holds at any strong minimizer. We now consider the right inequality in (5.1) for some particular choices of $B(x^*)$.

REMARK 5.2. *Assume that $\alpha(x)$ is continuous.*

(1) *For $B(x) = \nabla^2 f(x)$, any strong minimizer is a point of strong attraction if and only if $\alpha(x^*) \in (0, 2)$. In particular, any strong minimizer is a point of attraction of Newton's method ($\alpha(x) \equiv 1$) as is well known.*

(2) *For $B(x) = I$ (gradient method), any strong minimizer is a point of strong attraction if and only if $\alpha(x^*) < 2/\lambda_{\max}(\nabla^2 f(x^*))$. Moreover, we note the following fact.*

REMARK 5.3. *A minimizer x^* can be a point of weak repulsion if the Hessian matrix at x^* is not majorized by $2B(x^*)/\alpha(x^*)$.*

6. Nonlinear Least squares Problem. For the nonlinear least squares problem, we have

$$(6.1) \quad f(x) = \frac{1}{2} R^T(x) R(x).$$

where $R : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $m > n$, is twice continuously differentiable. The gradient and Hessian of $f(x)$ are, respectively,

$$(6.2) \quad \nabla f(x) = J(x)^T R(x) \quad \text{and} \quad \nabla^2 f(x) = J(x)^T J(x) + S(x),$$

where $J(x)$ is the Jacobian of $R(x)$ and

$$(6.3) \quad S(x) = \sum_{i=1}^m r_i(x) \nabla^2 r_i(x).$$

Consider the iteration (2.1) with $\alpha(x) = 1$ and

$$B(x) = J(x)^T J(x) + P(x).$$

In this case,

$$(6.4) \quad T(x) = x - (J(x)^T J(x) + P(x))^{-1} J(x)^T R(x),$$

and at any stationary point x^* of $f(x)$

$$(6.5) \quad T'(x^*) = (J(x^*)^T J(x^*) + P(x^*))^{-1} (P(x^*) - S(x^*)),$$

assuming continuity of $P(x)$ and nonsingularity of $J(x)^T J(x) + P(x)$ at x^* . Several well-known choices of $P(x)$ are the following:

1. Newton's method: $P(x) = S(x)$;
2. the Gauss-Newton method: $P(x) = 0$;
3. the Levenberg-Marquardt method: $P(x) = \mu(x)I$.

The Gauss-Newton method and the Levenberg-Marquardt method are popular choices for nonlinear least squares problems because they do not require second-order derivatives.

Now consider the iteration

$$(6.6) \quad x^{k+1} = T(x^k),$$

where $T(x)$ is defined in (6.4). The structure of least squares problem allows a simplification of Theorem 5.1.

THEOREM 6.1. *Let x^* be a stationary point of $f(x) = \frac{1}{2}R(x)^T R(x)$ where $f(x)$ is twice differentiable. Assume $J(x)^T J(x) + P(x)$ is continuous and symmetric positive definite at x^* . Then*

$$\rho(T'(x^*)) \leq 1$$

if and only if

$$(6.7) \quad -J(x^*)^T J(x^*) \preceq S(x^*) \preceq J(x^*)^T J(x^*) + 2P(x^*).$$

Moreover, $\rho(T'(x^)) < 1$ if and only if strict inequalities hold in (6.7).*

The right inequality in (6.7) says that the more “positive” $P(x^*)$ is, the more points of attraction the iteration may have. In view of this, we compare the Gauss-Newton method and the Levenberg-Marquardt method.

PROPOSITION 6.2. *Let x^* be a stationary point of $f(x) = \frac{1}{2}R(x)^T R(x)$ where $f(x)$ is twice differentiable and $J(x)$ has full column rank.*

1. *If x^* is a point of weak repulsion of the Levenberg-Marquardt method, it is also a point of weak repulsion of the Gauss-Newton method.*
2. *If x^* is a point of strong attraction of the Gauss-Newton method, it is also a point of strong attraction of the Levenberg-Marquardt method.*

The converses are not necessarily true whenever $\mu(x^) > 0$ in the Levenberg-Marquardt method.*

Analogous to Corollary 5.2, we also have the following.

COROLLARY 6.3. *Any stationary points x^* of $f(x) = \frac{1}{2}R(x)^T R(x)$ where the Hessian matrix has a negative eigenvalue, including all nondegenerate saddle points and maximizers where the Hessian is not the zero matrix, are points of weak repulsion of the Gauss-Newton method whenever $J(x^*)$ has full column rank. The same statement holds for the Levenberg-Marquardt method if either $J(x^*)$ has full column rank or $\mu(x^*) > 0$.*

It is known that iterates are generally repelled from saddle points in the Gauss-Newton method (see Björck [1], for example). It appears to us that the same property for the Levenberg-Marquardt method is not known.

7. Selective Minimization. Theorem 5.1 implies that a strong minimizer can be a point of strong attraction of the iteration (2.1) only if the corresponding Hessian matrix is majorized above by the matrix $2B(x^*)/\alpha(x^*)$.

In most applications, one would ideally like to find a global minimizer. Short of that, one would prefer local minimizers with low objective values. The fact that a given iterative method may turn certain minimizers into points of weak repulsion could be a useful tool for constructing algorithms whose iterates are attracted to desirable minimizers, but repelled from some undesirable minimizers.

To demonstrate this, we consider applying the Gauss-Newton and the Levenberg-Marquardt methods to minimization of nonlinear, nonconvex least squares problems where the global minimum value of the objective functions is zero or very small. For this type of problems, under mild conditions the global minimizers are points of strong attraction while local minimizers of high objective values are less likely to be points of strong attraction, as is illustrated by the following two lemmas.

LEMMA 7.1. *Let x^* be a strong minimizer of $f(x) = \frac{1}{2}R(x)^T R(x)$ where $f(x)$ is twice differentiable, $J(x)^T J(x) + P(x)$ is continuous and symmetric positive definite at x^* . Then x^* is a point of strong attraction of the iteration (6.6) if either $\nabla^2 r_i(x)$, $i = 1, 2, \dots, m$, are not all zero and*

$$(7.1) \quad \|R(x^*)\| < \frac{\lambda_{\min}[J(x^*)^T J(x^*) + 2P(x^*)]}{\sum_{i=1}^m \|\nabla^2 r_i(x^*)\|},$$

or $\|R(x^*)\| > 0$ and

$$(7.2) \quad \sum_{i=1}^m \|\nabla^2 r_i(x^*)\| < \frac{\lambda_{\min}[J(x^*)^T J(x^*) + 2P(x^*)]}{\|R(x^*)\|}.$$

Proof. It suffices to show that the strict inequalities hold in (6.7). Note that the left strict inequality in (6.7), i.e., $-J(x^*)^T J(x^*) \prec S(x)$, holds at any strong minimizer. Since

$$|\lambda_{\max}(S(x^*))| \leq \|S(x^*)\| \leq \|R(x^*)\| \left(\sum_{i=1}^m \|\nabla^2 r_i(x^*)\| \right),$$

the right strict inequality in (6.7), i.e., $S(x) \prec J(x^*)^T J(x^*) + 2P(x^*)$, holds if

$$\|R(x^*)\| \left(\sum_{i=1}^m \|\nabla^2 r_i(x^*)\| \right) < \lambda_{\min}[J(x^*)^T J(x^*) + 2P(x^*)],$$

which, under the respective conditions, leads to (7.1) and (7.2). \square

It is well-known that a strong minimizer x^* is a point of strong attraction of the Gauss-Newton method (or the Levenberg-Marquardt method) if either the residuals $r_i(x^*)$ or the Hessian matrices $\nabla^2 r_i(x^*)$, $i = 1, 2, \dots, m$, are sufficiently small (see Dennis and Steihaug [3], for example). The above lemma is an extension to a slightly more general setting.

Now let us define

$$\theta_i = r_i(x^*)/\|R(x^*)\|_1, \quad i = 1, 2, \dots, m,$$

and

$$(7.3) \quad C^* = \sum_{i=1}^m \theta_i \nabla^2 r_i(x^*).$$

Clearly, C^* is a linear combination of the Hessian matrices $\nabla^2 r_i(x^*)$, $i = 1, 2, \dots, m$, where the coefficients θ_i satisfy $|\theta_i| \in [0, 1]$ and $\sum_{i=1}^m |\theta_i| = 1$. To prove weak repulsion, an assumption on C^* is needed.

LEMMA 7.2. *Let x^* be a minimizer of $f(x) = \frac{1}{2}R(x)^T R(x)$ where $f(x)$ is twice differentiable and $J(x)^T J(x) + P(x)$ is continuous and symmetric positive definite. Assume further that $\lambda_{\max}(C^*) > 0$ where C^* is defined in (7.3). Then x^* is a point of weak repulsion of the iteration (6.6) if*

$$(7.4) \quad \|R(x^*)\|_1 > \frac{\lambda_{\max}(J(x^*)^T J(x^*) + 2P(x^*))}{\lambda_{\max}(C^*)},$$

Proof. We first note that $S(x^*) = \|R(x^*)\|_1 C^*$. A sufficient condition for x^* to be a point of weak repulsion of the iteration (6.6) is that

$$\lambda_{\max}(S(x^*)) = \|R(x^*)\|_1 \lambda_{\max}(C^*) > \lambda_{\max}(J(x^*)^T J(x^*) + 2P(x^*)),$$

which violates the right inequality in (6.7). Clearly, the above inequality is equivalent to (7.4) whenever $\lambda_{\max}(C^*) > 0$. \square

REMARK 7.1. *Lemma 7.1 provides a guarantee that any strong minimizer with sufficiently small residual value is a point of strong attraction of the iteration (6.6). On the other hand, Lemma 7.2 shows that minimizers with sufficiently large residual values will become a point of weak repulsion of the iteration (6.6) under some circumstances.*

We have done some numerical experiments on applying the Gauss-Newton and the Levenberg-Marquardt methods to global minimization of least squares problems where the optimal residual value is either zero or very small. Our numerical results have shown that the algorithms do skip some local minimizers, and have greater chances of converging to a global minimizer than, say, Newton's method which is attracted to any stationary point under mild conditions.

For more general problems, it is also possible to construct minimization algorithms that skip minimizers of high objective values while targeting lower-valued minimizers. For example, the following is a simple scheme:

$$B(x) = \begin{cases} I, & f(x) \geq \xi, \\ \nabla^2 f(x) + D(x), & \text{otherwise,} \end{cases}$$

where $D(x)$ is a diagonal matrix chosen to ensure $B(x) \succ 0$, and

$$\alpha(x) = \begin{cases} 2/\eta, & f(x) \geq \xi, \\ 1, & \text{otherwise,} \end{cases}$$

where $\eta > 0$. With these choices, the iteration

$$x^{k+1} = x^k - \alpha(x^k) B(x^k)^{-1} \nabla f(x^k)$$

will have the properties:

1. Any minimizer x^* with $f(x^*) \geq \xi$ and $\lambda_{\max}(\nabla^2 f(x^*)) > \eta$ is a point of weak repulsion.
2. Any strong minimizer x^* with $f(x^*) < \xi$ is a point of strong attraction.

Although we do not claim that the above construction is of any practical value, we do hope that combined with some random sampling techniques such as simulated annealing [4], the selective minimization property may lead to improved global optimization algorithms. This topic merits further study, but is outside the scope of this short paper. Instead, in the next section, we present a simple example showing the phenomenon of selective minimization.

8. Numerical Examples. In this section, we provide a couple of simple examples to illustrate the following points: (i) if $\{B^k\}$ is uniformly positive definite and $\{\alpha^k\}$ uniformly positive, then convergence to a point of weak repulsion seems to be highly unlikely in general; (ii) selective minimization does occur for certain problems. All our numerical experiments were done using Matlab.

8.1. First Example: Weak repulsion. We consider the following function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ (Levy and Gómez [5]):

$$(8.1) \quad f(x) = \sin^2(\pi y_1) + \sum_{i=1}^{n-1} (y_i - 1)^2 [1 + \sin^2(\pi y_{i+1})] + (y_n - 1)^2,$$

where

$$y_i = 1 + \frac{x_i - 1}{4}, \quad i = 1, 2, \dots, n,$$

and n is the number of variables in x . This function has many local minima but a unique global minimum at $x_i^* = 1, i = 1, 2, \dots, n$, where $f(x^*) = 0$.

We use the gradient method to construct an iteration

$$(8.2) \quad x^{k+1} = T(x^k) \equiv x^k - \alpha \nabla f(x^k)$$

and always choose

$$\alpha > \frac{2}{\lambda_{\max}(\nabla^2 f(x^*))}$$

so that at least one of the eigenvalues of $T'(x^*) \equiv I - \alpha \nabla^2 f(x^*)$ has an absolute value greater than one. By this very construction, the global minimizer x^* is a point of weak repulsion of the iteration (8.2) since $|\lambda_{\max}(T'(x^*))| > 1$.

We applied iteration (8.2) to problem (8.1) for $n = 2, 3, 10, 50, 100$. The actual values of the steplength α vary with n and are not of interest here. For each n value, we selected 100 random starting points close to x^* , namely

$$x^1 = x^* + \epsilon(\text{rand}(n, 1) - 0.5),$$

where $\epsilon = 10^{-3}$ and **rand** is the Matlab command for generating a uniformly distributed random n -vector with components in $[0, 1]$. The stopping criterion used in our experiments is that either $\|\nabla f(x^k)\| < 10^{-14}$ or the number of iterations reaches 100.

In all of our numerical experiments, we did not obtain a single case of convergence to a point of weak repulsion. These experiments give a rather strong indication that convergence to a point of weak repulsion may be improbable in general.

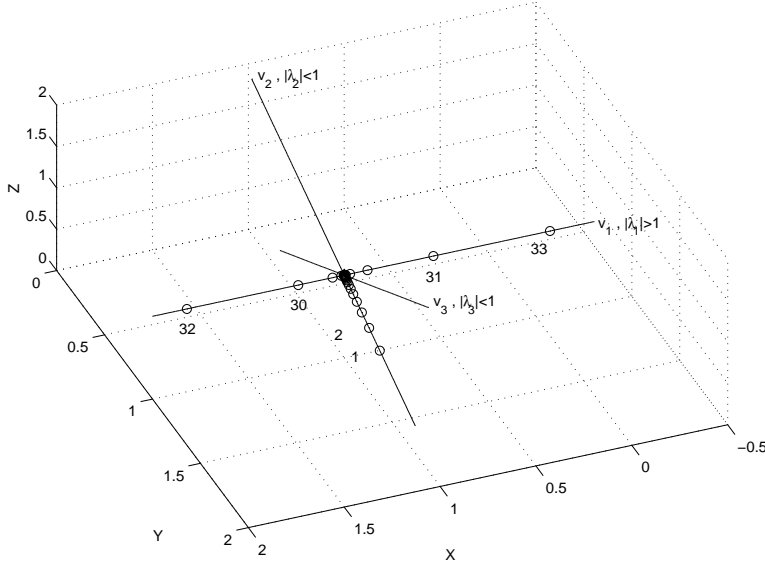
In Figure 1, we present a specific example for $n = 3$ and

$$\alpha = \frac{3}{\lambda_{\max}(\nabla^2 f(x^*))} = 4.3061.$$

For this choice of α , the three eigenvalues of $T'(x^*)$ are

$$\lambda_1 = -2, \quad \lambda_2 = \lambda_3 = 0.7182.$$

In order to dramatize the situation, we choose a starting point $x^1 = (1, 1.3709, 0.6647)$ so that $x^1 - x^*$ is in the direction of v_2 — the eigenvector direction corresponding to

FIG. 8.1. *Non-convergence to a point of weak repulsion*

the eigenvalue $\lambda_2 = 0.7182$. In the picture, the small circles represent the positions of the iterates, and the numbers beside the circles are the iteration numbers. As one can see, initially the iterates approach x^* along the direction of v_2 . However, as the iterates get closer to x^* (with $\|\nabla f(x)\| \approx 10^{-4}$), unable to stay in the direction of v_2 they start to drift away from x^* along the direction of v_1 , which is the eigenvector direction corresponding to the eigenvalue $\lambda_1 = -2$.

8.2. Second Example: Selective Minimization. We now consider the following two-dimensional least squares problem

$$(8.3) \quad f(x, y) = \frac{1}{2} R(x, y)^T R(x, y),$$

where, for $\alpha = 1.2$ and $\beta = 6$,

$$(8.4) \quad R(x, y) = \begin{pmatrix} \alpha \sin(\pi(1 + x/4)) \\ \beta(x/4)[1 + \alpha^2 \sin^2(\pi(1 + y/4))]^{1/2} \\ y/4 \\ \alpha \sin(\pi(1 + y/4)) \\ \beta(y/4)[1 + \alpha^2 \sin^2(\pi(1 + x/4))]^{1/2} \\ x/4 \end{pmatrix}.$$

This function $f(x, y)$ is symmetric about both the x -axis and the y -axis, and has a unique global minimizer at the origin with zero-residual. We will concentrate our attention to the square: $-5 \leq x, y \leq 5$, which will be considered to be the area of our interest. In this square, the function has four local minimizers at

$$(x^*, y^*) \approx (\pm 3.64, \pm 3.64)$$

with relatively high residual value $f(x^*, y^*) \approx 34.09$. The function also has four saddle points in the square of interest at

$$(x^*, y^*) \approx (\pm 2.98, \pm 2.98)$$

with residual value $f(x^*, y^*) \approx 36.12$. See Figure 2 for a plot of $f(x, y)$ in the square of interest.

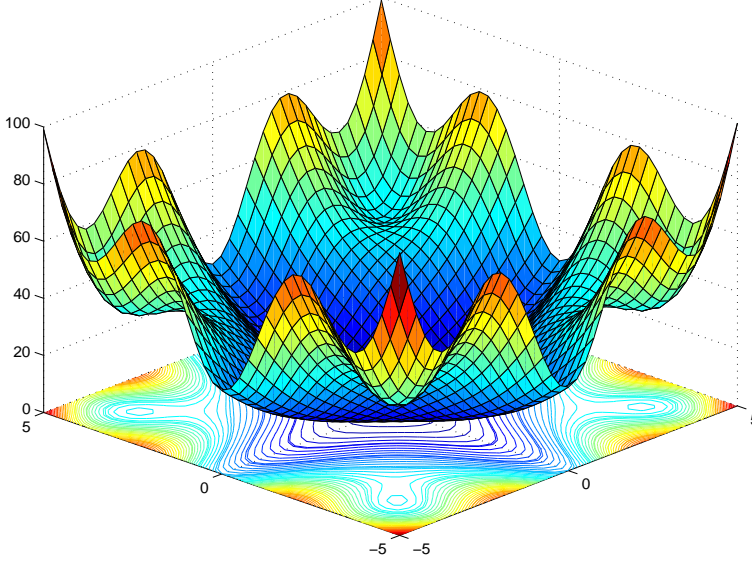


FIG. 8.2. *The 2-dimensional Test Function*

We apply the Gauss-newton method, i.e., the iteration (6.6) with $P(x) = 0$ in (6.4), to minimizing $f(x, y)$ defined in (8.3) and (8.4). In our experiments, we have found that the Gauss-newton method is always well defined in the square of interest.

From Lemma 7.1, we know that the global minimizer at the origin is a point of strong attraction for the Gauss-Newton iteration. On the other hand, our calculation shows that for the Gauss-Newton iteration, $\lambda_i(T'(x))$, $i = 1, 2$, are, respectively and approximately -16.86 and -2.29 at the four local minimizers. Therefore, they are points of strong repulsion. The saddle points are nondegenerate and hence points of weak repulsion of the Gauss-Newton iteration. In fact, (4.1) holds at the saddle points which means that they are not points of strong repulsion.

For the purpose of comparison, we also apply the Levenberg-Marquardt method and the Newton method to the problem as well. For the Levenberg-Marquardt method, we choose $P(x) = 10I$ in (6.4). With this choice, all minimizers in the square, global or local, are points of strong attraction, and the saddle points remain points of weak repulsion where (4.1) holds. On the other hand, all the stationary points in the square are points of strong attraction of the Newton method.

We run the three methods starting from the following grid of initial points in the first quadrant:

$$(x_i, y_j) = (i, j)/4, \quad 0 \leq i, j \leq 20.$$

Since the function is symmetric about both axes, we can duplicate the behavior of the methods in the first quadrant in the other three quadrants. For each method and each initial point, we record whether or not the iterates converge to the global minimizer at the origin, or to one of the other stationary points (some may be outside of the square of interest), or do not converge within a prescribed maximum number of

iterations, which is set to 100 in our experiments. The convergence criterion is that the norm of the gradient be less than 10^{-8} .

We summarize the numerical results for the three methods below.

1. **Gauss-Newton:** From all the starting points without exception, the Gauss-Newton method converged to the global minimizer at the origin. We note that never did any starting point lead to a point of weak repulsion (saddle point) no matter how close it was.
2. **Levenberg-Marquardt:** With the particular choice of $P(x) = 10I$ for the Levenberg-Marquardt method, all the starting points led to one of the five minimizers in the square, with around 75% to the global minimizer and the rest 25% to the local ones. Again, never did a starting point lead to a saddle point.
3. **Newton:** For the Newton method, about 50% of the starting points led to the global minimizer, and about 30% to other stationary points in the square. The rest of points either led to stationary points outside the square, or were such that the method did not terminate after 100 iterations.

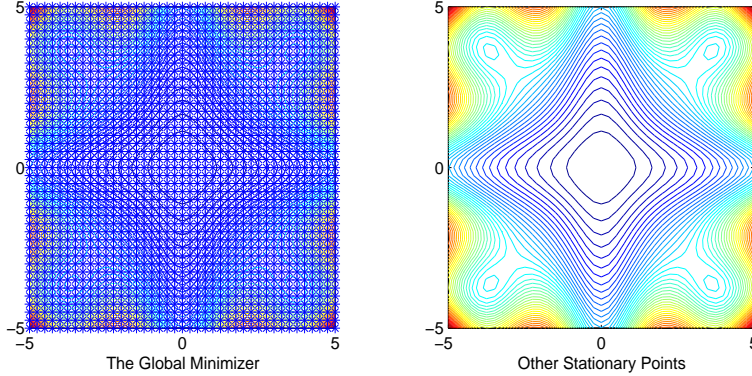


FIG. 8.3. *Estimated Regions of Attraction for the Gauss-Newton Method*

In Figures 3, 4 and 5, we plot the (estimated) region of attraction of the global minimizer and the combined region of attraction of all the other stationary points in the square for the three methods, respectively. The asterisks represent points from which a method converged to the global minimizer (in the pictures on the left) or to one of the other stationary points inside the square (in the pictures on the right). On the background, we also plot the contour of the test function.

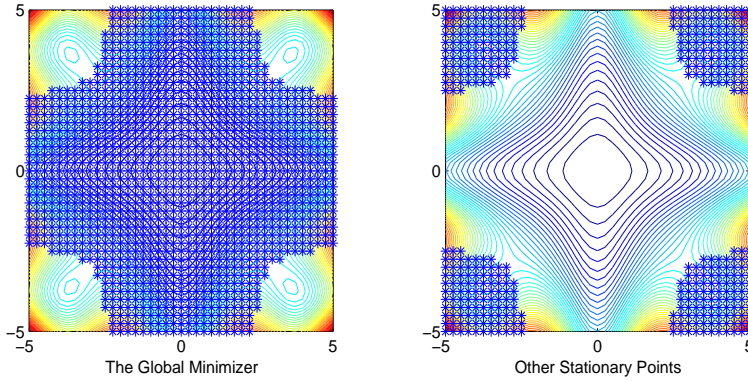
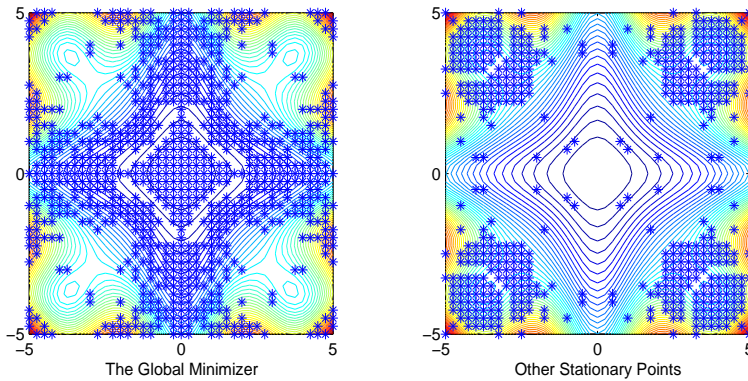
In the picture on the right side of Figure 5, it appears that at each corner an area of attraction of the local minimizer is separated by a narrow band from an area of attraction of the nearby saddle point.

9. Final Remarks. For the general iteration process

$$x^{k+1} = x^k - \alpha^k (B^k)^{-1} \nabla f(x^k),$$

Theorem 5.1 has several interesting, but previously unnoticed, implications. We consider the following two observations to be particularly worthwhile.

Firstly, as long as one keeps $\{B^k\}$ uniformly positive definite and $\{\alpha^k\}$ bounded away from zero, then the undesirable case of converging to a saddle point should not be of general concern.


 FIG. 8.4. *Estimated Regions of Attraction for the Levenberg-Marquardt Method*

 FIG. 8.5. *Estimated Regions of Attraction for the Newton Method*

Secondly, if one does not always enforce descent, then under favorable conditions a method can actually generate iterates that skip some undesirable minimizers while still being attracted to more desirable minimizers.

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