Chapter 4

Matrix Secant Methods

4.1 Equation Solving

In this section we again study the problem of finding \( \bar{\mathbf{x}} \in \mathbb{R}^n \) such that \( g(\bar{\mathbf{x}}) = 0 \) where \( g : \mathbb{R}^n \to \mathbb{R}^n \) is \( C^1 \). Specifically, we will consider Newton-Like methods of a special type. Recall that in a Newton-Like method the iteration scheme takes the form

\[
x_{k+1} := x_k - M_k^{-1}g(x_k),
\]

where \( M_k \) is meant to approximate \( g'(x_k) \). In the one dimensional case, a choice of particular note is the secant approximation

\[
M_k = \frac{g(x_{k-1}) - g(x_k)}{x_{k-1} - x_k}.
\]

With this approximation one has

\[
g'(x_k)^{-1} - M_k^{-1} = \frac{g(x_{k-1}) - [g(x_k) + g'(x_k)(x_{k-1} - x_k)]}{g'(x_k)[g(x_{k-1}) - g(x_k)]}.
\]

Also, near a point \( x^* \) at which \( g' \) is non-singular there exists an \( \alpha > 0 \) such that

\[
\alpha \| x - y \| \leq \| g(x) - g(y) \|.
\]

Consequently, by the Quadratic Bound Lemma,

\[
\| g'(x_k)^{-1} - M_k^{-1} \| \leq \frac{K}{\alpha \| g'(x_k) \| \| x_{k-1} - x_k \|} \frac{1}{\| x_{k-1} - x_k \|} \leq K \| x_{k-1} - x_k \|
\]

for some constant \( K > 0 \) whenever \( x_k \) and \( x_{k-1} \) are sufficiently close to \( x^* \). Therefore, by Theorem 2.3.1, there secant method is locally two step quadratically convergent to a non-singular solution of the equation \( g(x) = 0 \). An additional advantage of this approach is that no extra function evaluations are required to obtain the approximation \( M_k \).
Unfortunately, the secant approximation (4.1.2) is meaningless in the \( n > 1 \) dimensional case since division by vectors is undefined. However, this can be rectified by simply writing

\[
M_k(x_{k-1} - x_k) = g(x_{k-1}) - g(x_k).
\]

Equation (4.1.3) is called the Quasi-Newton equation (QNE) at \( x_k \) and it determines \( M_k \) along an \( n \) dimensional manifold in \( \mathbb{R}^{n \times n} \). Thus equation (4.1.3) is not enough to uniquely determine \( M_k \) since (4.1.3) is \( n \) linear equations in \( n^2 \) unknowns. Consequently, we may place further conditions on the update \( M_k \) if we wish to do so. In order to see what further properties one would like the update to possess, let us consider an overall iteration scheme based on (4.1.1). At every iteration we have \((x_k, M_k)\) and compute \( x_{k+1} \) by (4.1.1). Then \( M_{k+1} \) is constructed to satisfy (4.1.3). If \( M_k \) is close to \( g'(x_k) \) and \( x_{k+1} \) is close to \( x_k \), then \( M_{k+1} \) should be chosen not only to satisfy (4.1.3) but also to be as “close” to \( M_k \) as possible.

In what sense should we mean “close” here? In order to facilitate the computations it is reasonable to mean “algebraically” close in the sense that \( M_{k+1} \) is only a rank 1 modification of \( M_k \), i.e. there are vectors \( u, v \in \mathbb{R}^n \) such that

\[
M_{k+1} = M_k + uv^T.
\]

Multiplying (1.3) by

\[
s_k := x_{k+1} - x_k
\]

and using (4.1.3) we find that

\[
y_k = M_{k+1}s_k = M_k s_k + uv^Ts_k
\]

where \( y_k := g(x_{k+1}) - g(x_k) \). Hence, if \( v^Ts_k \neq 0 \), we obtain

\[
u = \frac{y_k - M_k s_k}{v^Ts_k}
\]

and

\[
M_{k+1} = M_k + \frac{(y_k - M_k s_k)v^T}{v^Ts_k}.
\]

Equation (4.1.5) determines a whole class of rank one updates that satisfy the QNE where one is allowed to choose \( v \in \mathbb{R}^n \) as long as \( v^Ts_k \neq 0 \). If \( s_k \neq 0 \), then an obvious choice for \( v \) is \( s_k \) yielding the update

\[
M_{k+1} = M_k + \frac{(y_k - M_k s_k)s_k^T}{s_k^Ts_k}.
\]

This is known as Broyden’s update. Given the algebraically “close” updates in (4.1.5), it is reasonable to ask whether there related updates that are analytically close.

**Theorem 4.1.1** Let \( A \in \mathbb{R}^{n \times n}, s, y \in \mathbb{R}^n, s \neq 0 \). Then for any matrix norms \( \| \cdot \| \) and \( \| \cdot \| \) such that

\[
\| AB \| \leq \| A \| \| B \|
\]
4.1. EQUATION SOLVING

and

\[ \| \frac{vv^\tau}{v^\tau v} \| \leq 1, \]

the solution to

\[ (4.1.7) \quad \min\{\|B - A\| : Bs = y\} \]

is

\[ (4.1.8) \quad A_+ = A + \frac{(y - As)s^\tau}{s^\tau s}. \]

In particular, (4.1.8) solves (4.1.7) when \( \| \cdot \| \) is the \( \ell_2 \) matrix norm, and (4.1.8) solves (4.1.7) uniquely when \( \| \cdot \| \) is the Frobenius norm.

**Proof:** Let \( B \in \{B \in \mathbb{R}^{n \times n} : Bs = y\} \), then

\[ \|A_+ - A\| = \| \frac{(y - As)s^\tau}{s^\tau s} \| = \|(B - A) \frac{s s^\tau}{s^\tau s}\| \leq \|B - A\| \| \frac{s s^\tau}{s^\tau s}\| \leq \|B - A\|. \]

Note that if \( \| \cdot \| = \| \cdot \|_2 \), then

\[ \| \frac{vv^\tau}{v^\tau v} \|_2 = \sup \{ \| \frac{vv^\tau}{v^\tau v}x \|_2 : \|x\|_2 = 1 \} \]

\[ = \sup \{ \sqrt{\frac{(v^\tau x)^2}{\|v\|^2}} : \|x\|_2 = 1 \} \]

\[ = 1, \]

so that the conclusion of the result is not vacuous. For uniqueness observe that the Frobenius norm is strictly convex and \( \|A \cdot B\|_F \leq \|A\|_F \|B\|_2 \).

Therefore, the Broyden update (4.1.6) is both algebraically and analytically close to \( M_k \). These properties indicate that it should perform well in practice and indeed it does.

**Algorithm: Broyden’s Method**

Initialization: \( x_0 \in \mathbb{R}^n, M_0 \in \mathbb{R}^{n \times n} \)

Having \( (x_k, M_k) \) compute \( (x_{k+1}, M_{k+1}) \) as follows:

Solve \( M_k s_k = -g(x_k) \) for \( s_k \) and set

\[ x_{k+1} : = x_k + s_k \]

\[ y_k : = g(x_k) - g(x_{k+1}) \]

\[ M_{k+1} : = M_k + \frac{(y_k - M_k s_k s_k^\tau)}{s_k^\tau s_k}. \]

Due to its derivation we call methods based up (4.1.5) matrix secant methods. In the literature they are also called Quasi-Newton methods.
Observe that the derivation of (4.1.5) only relied upon the relations
\[ M_{k+1}s_k = y_k \]
and
\[ M_{k+1} = M_k + uv^T. \]
Thus by switching the roles of \( s_k \) and \( y_k \) it is possible to obtain an inverse updating scheme. That is if instead of (4.1.1) we write
\[ x_{k+1} := x_k - W_k g(x_k) \]
where \( W_k \approx [g'(x_k)]^{-1} \), then a matrix secant method for updating \( W_k \) would be
\[
W_{k+1} := W_k + \frac{(s_k - W_k y_k) y_k^T}{y_k^T y_k},
\]
since we want the QNE
\[ x_{k+1} - x_k = s_k - W_{k+1} y_k = W_{k+1} (g(x_{k+1}) - g(x_k)) \]
to hold. It would be interesting to determine if \( W_k = M_k^{-1} \). For this we require the following well-known lemma.

**Lemma 4.1.1 (Sherman-Morrison-Woodbury)** Suppose \( A \in \mathbb{R}^{n \times n} \), \( U \in \mathbb{R}^{n \times k} \), \( V \in \mathbb{R}^{n \times k} \) are such that both \( A^{-1} \) and \( (I + V^T A^{-1} U)^{-1} \) exist, then
\[
(A + U V^T)^{-1} = A^{-1} - A^{-1} U (I + V^T A^{-1} U)^{-1} V^T A^{-1}
\]

**Exercise:** Prove Lemma 4.1.1.

The above lemma verifies that if \( M^{-1} \) exists and \( s^T M^{-1} y \neq 0 \), then
\[
[M + \frac{(y - Ms)s^T}{s^T s}]^{-1} = M^{-1} + \frac{(s - M^{-1} y)s^T M^{-1}}{s^T M^{-1} y}.
\]
Consequently, it is not true that the \( W_k \)'s obtained from (4.1.9) and the \( M_k \)'s from (4.1.6) satisfy
\[ W_k = M_k^{-1}. \]
However, (4.1.10) does indicate a variation on both (4.1.6) and (4.1.9). Specifically, in (4.1.5) one could choose \( v = M_k y_k \), in which case one does obtain the inverse of (4.1.9). Conversely, one could replace (4.1.9) with
\[
W_{k+1} := W_k + \frac{(s_k - W_k y_k) s_k^T W_k}{s_k^T W_k y_k}
\]
yielding the inverse of (4.1.6).
4.2. MINIMIZATION

On the surface computing the inverse updates appears to be more attractive since then we need not solve the equation

\[ B_k s_k = y_k \]

for \( s_k \) at every iteration. However, this approach can suffer from fatal numerical instabilities if \( g'(x^*) \) is singular or nearly singular.

Although we do not pause to establish the convergence rates here, we do give the following result due to Dennis and Moré (1974).

**Theorem 4.1.2** Let \( g : \mathbb{R}^n \rightarrow \mathbb{R}^n \) be continuously differentiable in an open convex set \( D \subset \mathbb{R}^n \). Assume that there exists \( x^* \in \mathbb{R}^n \) and \( r, \beta > 0 \) such that \( x^* + rB \subset D \), \( g(x^*) = 0 \), \( g'(x^*)^{-1} \) exists with \( \| g'(x^*)^{-1} \| \leq \beta \), and \( g' \) is Lipschitz continuous on \( x^* + rB \) with Lipschitz constant \( \gamma > 0 \). Then there exist positive constants \( \epsilon \) and \( \delta \) such that if \( \| x_0 - x^* \| \leq \epsilon \) and \( \| B_0 - g'(x_0) \| \leq \delta \), then the sequence \( \{ x_k \} \) generated by the iteration

\[
\begin{align*}
  x_{k+1} & := x_k + s_k \text{ where } s_k \text{ solves } 0 = g(x_k) + B_k s \\
  B_{k+1} & := B_k + \frac{(y_k - B_k s_k)s_k^T}{s_k^T s_k} \text{ where } y_k = g(x_{k+1}) - g(x_k)
\end{align*}
\]

is well-defined with \( x_k \rightarrow x^* \) superlinearly.

4.2 Minimization

In this section the underlying problem is one of minimization:

\[ \mathcal{P} : \text{minimize } f(x) \]

where \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) is \( C^2 \). The basic idea is to modify and/or extend the matrix secant methods of the previous section to the setting of minimization where one wishes to solve the equation \( \nabla f(x) = 0 \). In this context the QNE becomes

\[ M_{k+1} s_k = y_k \]

where \( s_k := x_{k+1} - x_k \) and

\[ y_k := \nabla f(x_{k+1}) - \nabla f(x_k). \]

A straightforward application of Broyden’s method would yield the update

\[ M_{k+1} = M_k + \frac{(y_k - M_k s_k)s_k^T}{s_k^T s_k}. \]

However, this is unsatisfactory for two reasons:

1. Since \( M_k \) is intended to approximate \( \nabla^2 f(x_k) \) it is desirable that \( M_k \) be symmetric.
2. Since we are concerned with minimization, then at least locally one can assume the second order sufficiency condition holds. Consequently, we would like the $M_k$’s to be positive definite.

To address problem 1 above, one could return to equation (4.1.5) for an alternate update that preserves symmetry. Such an update is uniquely obtained by setting

$$v = (y_k - M_k s_k).$$

This is called the symmetric rank 1 update or SR1. Although this update can on occasion exhibit problems with numerical stability, it has recently received a great deal of renewed interest. The stability problems occur whenever

$$v^T s_k = \nabla f(x_k)^T M_k^{-1} (\nabla f(x_k) - \nabla f(x_{k+1}))$$

tends to zero faster than $\|\nabla f(x_k)\|^2$.

The following alternate strategy has been proposed by Powell. One begins by symmetrizing the Broyden update

$$M_1 = M + \frac{(y - Ms)s^T}{s^Ts}.$$

This is done by replacing $M_1$ with its symmetric part

$$M_2 = \frac{1}{2}(M_1 + M_1^T).$$

But then the QNE fails. To remedy this set

$$M_3 = M_2 + \frac{(y - M_2 s)s^T}{s^Ts}.$$

But again symmetry fails so set

$$M_4 = \frac{1}{2}(M_3 + M_3^T).$$

Proceeding in this way we get a sequence $\{M_k\}$ with

$$\begin{cases} M_{2k+1} = M_{2k} + \frac{(y - M_{2k}s)s^T}{s^Ts} \\ M_{2(k+1)} = \frac{1}{2}(M_{2k+1} + M_{2k+1}^T) \end{cases}$$

for $k = 0, 1, \ldots$. Since the set $S_1 = \{M \in \mathbb{R}^{n \times n} : Ms = y\}$ is an affine subset of $\mathbb{R}^{n \times n}$ and the set $S_2 = \{M \in \mathbb{R}^{n \times n} : M$ is symmetric\} is a subspace of $\mathbb{R}^{n \times n}$, and the equations (4.2) represent a sequence of alternating orthogonal projections in $\mathbb{R}^{n \times n}$ onto $S_1$, and $S_2$ respectively, the sequence $\{M_k\}$ must converge to a fixed point solving the proximation problem

$$\min \|M - M\|_F$$

subject to $M \in S_1, (M - M) \in S_2$. 

CHAPTER 4. MATRIX SECANT METHODS
4.2. MINIMIZATION

It is possible to show that the solution is

\[
\overline{M} = M + \frac{(y - Ms)s^\tau + s(y - Ms)^\tau}{s^\tau s} - \frac{(y - Ms)^\tau sss^\tau}{(s^\tau s)^2}.
\]

The update (4.2.12) is called the Powell-symmetric-Broyden (PSB) update.

Update (4.2.12) was derived to preserve both symmetry and stability, however there is no guarantee that if \( M \) is positive definite, then \( \overline{M} \) is also. We now address the question of when this is possible. That is, suppose \( M \in \mathbb{R}^{n \times n} \) symmetric and positive definite, we wish to find \( \overline{M} \) satisfying the QNE such that \( \overline{M} \) is also symmetric and positive definite. Let \( M = LL^\tau \) be the Cholesky factorization of \( M \). If \( \overline{M} \) is to be symmetric and positive definite then there is a matrix \( J \in \mathbb{R}^{n \times n} \) such that \( \overline{M} = JJ^\tau \). The QNE implies that if

\[
J^\tau s = v
\]
then

\[
Jv = y.
\]

Let us try to apply the Broyden update technique to (4.2.14), \( J \), and \( L \). That is, suppose that

\[
J = L + \frac{(y - Lv)v^\tau}{v^\tau v}.
\]

Then by (4.2.13)

\[
v = J^\tau s = L^\tau s + \frac{v(y - Lv)^\tau s}{v^\tau v}.
\]

This expression implies that \( v \) must have the form

\[
v = \alpha L^\tau s
\]
for some \( \alpha \in \mathbb{R} \). Substituting this back into (4.2.16) we get

\[
\alpha L^\tau s = L^\tau s + \frac{\alpha L^\tau s(y - \alpha LL^\tau s)^\tau s}{\alpha^2 s^\tau LL^\tau s}.
\]

Hence

\[
\alpha^2 = \left[ \frac{s^\tau y}{s^\tau Ms} \right].
\]

Consequently, such a matrix \( J \) satisfying (4.2.16) exists only if \( s^\tau y > 0 \) in which case

\[
J = L + \frac{(y - \alpha Ms)s^\tau L}{\alpha s^\tau Ms},
\]

with

\[
\alpha = \left[ \frac{s^\tau y}{s^\tau Ms} \right]^{1/2},
\]
yielding
\[
\overline{M} = M + \frac{yy^T}{y^Ts} - \frac{Ms^TM}{s^TMs}.
\]
Moreover, the Cholesky factorization for \(\overline{M}\) can be obtained directly from the matrices \(J\). Specifically, if the QR factorization of \(J^T\) is \(J^T = QR\), we can set \(\overline{L} = R\) yielding
\[
\overline{M} = JJ^T = R^TQR = \overline{L}\overline{L}^T.
\]

The question of course remains as to how one can assure the positivity of the product \(s^T y\). Recall that in the iterative context
\[
s = s_k = -\lambda_k M_k^{-1} \nabla f(x_k)
\]
and
\[
y = y_k = \nabla f(x_{k+1}) - \nabla f(x_k).
\]
Hence
\[
y^Ts = y_k^Ts_k = \nabla f(x_{k+1})^Ts_k - \nabla f(x_k)^Ts_k = \lambda_k \nabla f(x_k + \lambda_k d_k)^Td_k - \lambda_k \nabla f(x_k)^T k_k,
\]
where \(d_k := -M_k^{-1} \nabla f(x_k)\). Now since \(M_k\) is positive definite the direction \(d_k\) is a descent direction for \(f\) at \(x_k\) and so \(\lambda_k > 0\). Therefore, to assure that \(y^Ts > 0\) we need only show that we can choose \(\lambda_k > 0\) so that
\[
(4.2.18) \quad \nabla f(x_k + \lambda_k d_k)^Td_k \geq \beta \nabla f(x_k)^Td_k
\]
for some \(\beta \in (0,1)\).

Note that for any descent direction \(d\) of \(f\) at \(x_k\) we can choose
\[
\overline{\lambda} := \text{arg min}\{f(x_k + \lambda d) : \lambda > 0\}
\]
in which case \(\overline{\lambda} = +\infty\) or
\[
\nabla f(x_k + \overline{\lambda} d)^Td = 0.
\]
Therefore, \(\lambda_k\) can always be chosen to make \(y_k^Ts_k > 0\), and so the updating strategy (4.2.17) can be used to guarantee both symmetry and positive definiteness if a suitable line search is employed. We return to the question of what a suitable line search is later in this section.

The update (4.2.17) is called the BFGS (Broyden-Fletcher-Goldfarb-Shanno) update and is currently considered the best available matrix secant type update for minimization. Observe in (4.2.17) that if both \(\overline{M}\) and \(M\) are positive definite, then they are both invertible. The Sherman-Morrison-Woodbury formula shows that the inverse is given by
\[
\overline{M}^{-1} = M^{-1} + \frac{(s - M^{-1}y)s^T + s(s - M^{-1}y)^T}{y^Ts} - \frac{(s - M^{-1}y)^Tyss^T}{(y^Ts)^2}.
\]
Thus the corresponding inverse updating scheme for the BFGS update is

\[
\bar{W} = W + \frac{(s - Wy)s^\tau + s(s - Wy)^\tau}{y^\tau s} - \frac{(s - Wy)^\tau y ss^\tau}{(y^\tau s)^2}.
\]

One can now use this representation of the inverse to write down an alternate update of \( M \), it is

\[
\hat{M} = M + \frac{(y - Ms)y^\tau + y(y - Ms)^\tau}{y^\tau s} - \frac{(y - Ms)^\tau yy^\tau}{(y^\tau s)^2}.
\]

This is known as the DFP formula named after Davidon-Fletcher-Powell.

One can show that the DFP, BFGS, and SR1 updates are all members of a one parameter family of updates known as the Broyden family. In order to see this set

\[
a := s^\tau Ms, \ b := y^\tau s, \ c := y^\tau Wy,
\]

and, assuming \( a, b, \) and \( c \) are nonzero, define two vectors

\[
m := \frac{y}{b} - \frac{Ms}{a}
\]

and

\[
w := \frac{s}{b} - \frac{Wy}{c}
\]

satisfying \( m^\tau s = 0 = w^\tau y \). Then define two parameterized families of matrices by

\[
\bar{M}(\mu) := M - \frac{Mss^\tau M}{a} + \frac{yy^\tau}{b} + \mu mm^\tau,
\]

and

\[
\bar{W}(\nu) := W - \frac{Wyy^\tau W}{c} + \frac{ss^\tau}{b} + \nu ww^\tau.
\]

The following table illustrates the relationship between the updates and various values of \( \mu \) and \( \nu \):

<table>
<thead>
<tr>
<th>Update</th>
<th>( \mu )</th>
<th>( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFP</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>BFGS</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>SR1</td>
<td>( b/(b - a) )</td>
<td>( b/(b - c) )</td>
</tr>
</tbody>
</table>

We now turn to the study of an appropriate line search procedure. In particular, this procedure should enforce inequality (4.2.18). The line search that we consider is a combination of the Armijo-Goldstein procedure and (4.2.18).
Lemma 4.2.1 Let \( f : \mathbb{R}^n \to \mathbb{R} \) be \( C^1 \) and let \( x, d \in \mathbb{R}^n \) be given so that \( \nabla f(x)^T d < 0 \) and the set \( \{ f(x + \lambda d) : \lambda > 0 \} \) is bounded below. Then for every choice of the scalars \( 0 < c < \beta < 1 \) the set
\[
\left\{ \lambda > 0 \left| f(x + \lambda d) - f(x) \leq c \lambda \nabla f(x)^T d, \text{ and } \nabla f(x + \lambda d)^T d \geq \beta \nabla f(x)^T d \right. \right\}
\]
is non-empty.

Exercise: Prove Lemma 4.2.1.

Thus it is possible to choose a steplength \( \lambda \) such that both the Armijo inequality
\[
f(x + \lambda d) - f(x) \leq c \lambda \nabla f(x)^T d
\]
and inequality (4.2.18) are satisfied. Concerning this steplength Powell [1976] has established the following convergence result.

Theorem 4.2.1 Let \( f : \mathbb{R}^n \to \mathbb{R} \) be \( C^2 \). Assume that

1. \( \nabla^2 f \) is Lipschitz continuous, and
2. \( \nabla^2 f \) is strongly convex.

Let \( x_0 \in \mathbb{R}^n \), \( H_0 \in \mathbb{R}^{n \times n} \) symmetric and positive definite, and \( \{ x_k \} \) be a sequence defined by
\[
s_k := -M_k^{-1} \nabla f(x_k), \quad x_{k+1} = x_k + \lambda_k s_k
\]
where \( \lambda_k \) is chosen from the set defined in (4.2.21) with \( \lambda_k = 1 \) being used whenever it is a permissible value, and \( M_{k+1} \) is defined as the BFGS update
\[
M_{k+1} := M_k + \frac{y_k y_k^T}{y_k^T s_k} - \frac{M_k s_k^T s_k}{s_k^T H_k s_k}.
\]
Then the sequences \( \{ x_k \} \) and \( \{ M_k \} \) are well defined and \( \{ x_k \} \) converges \( q \)-superlinearly to \( \bar{x} \) the unique point at which \( f \) attains its global minimum value.

We omit the proof of the above result as it is rather involved. It may be found in


We mention though that it is still an open problem as to whether a similar result holds for the DFP update.

The variable metric methods discussed in this section are by far the methods of choice for most unconstrained optimization problems when good derivative approximations are available. Observe that one could employ the PSB, BFGS, or DFP formulas to do inverse
updating, but in general this is not done due to possible numerical instabilities that can arise when the hessians are nearly singular. If one wishes to investigate these methods further an excellent survey article is


also see