

based on the Wolfe conditions (3.6) or strong Wolfe conditions (3.7), so that BFGS updating is stable.

The limited-memory BFGS algorithm can be stated formally as follows.

Algorithm 7.5 (L-BFGS).

Choose starting point x_0 , integer $m > 0$;
 $k \leftarrow 0$;
repeat
 Choose H_k^0 (for example, by using (7.20));
 Compute $p_k \leftarrow -H_k \nabla f_k$ from Algorithm 7.4;
 Compute $x_{k+1} \leftarrow x_k + \alpha_k p_k$, where α_k is chosen to
 satisfy the Wolfe conditions;
 if $k > m$
 Discard the vector pair $\{s_{k-m}, y_{k-m}\}$ from storage;
 Compute and save $s_k \leftarrow x_{k+1} - x_k$, $y_k = \nabla f_{k+1} - \nabla f_k$;
 $k \leftarrow k + 1$;
until convergence.

The strategy of keeping the m most recent correction pairs $\{s_i, y_i\}$ works well in practice; indeed no other strategy has yet proved to be consistently better. During its first $m - 1$ iterations, Algorithm 7.5 is equivalent to the BFGS algorithm of Chapter 6 if the initial matrix H_0 is the same in both methods, and if L-BFGS chooses $H_k^0 = H_0$ at each iteration.

Table 7.1 presents results illustrating the behavior of Algorithm 7.5 for various levels of memory m . It gives the number of function and gradient evaluations (nfg) and the total CPU time. The test problems are taken from the CUTE collection [35], the number of variables is indicated by n , and the termination criterion $\|\nabla f_k\| \leq 10^{-5}$ is used. The table shows that the algorithm tends to be less robust when m is small. As the amount of storage increases, the number of function evaluations tends to decrease; but since the cost of each iteration increases with the amount of storage, the best CPU time is often obtained for small values of m . Clearly, the optimal choice of m is problem dependent.

Because some rival algorithms are inefficient, Algorithm 7.5 is often the approach of choice for large problems in which the true Hessian is not sparse. In particular, a Newton

Table 7.1 Performance of Algorithm 7.5.

Problem	n	L-BFGS $m = 3$		L-BFGS $m = 5$		L-BFGS $m = 17$		L-BFGS $m = 29$	
		nfg	time	nfg	time	nfg	time	nfg	time
DIXMAANL	1500	146	16.5	134	17.4	120	28.2	125	44.4
EIGENALS	110	821	21.5	569	15.7	363	16.2	168	12.5
FREUROTH	1000	>999	—	>999	—	69	8.1	38	6.3
TRIDIA	1000	876	46.6	611	41.4	531	84.6	462	127.1