Practical Optimization Algorithms
实用优化算法

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Chapter V: Quasi-Newton Methods (拟牛顿法)

Outline

- The DFP (Davidon, Fletcher and Powell)
- The BFGS (Broyden, Fletcher, Goldfarb and Shanno)
- The SR1 (Symmetric-Rank-1)
- The Broyden Class (DFP+BFGS)
- Convergence Analysis

The DFP Method

- The approaching quadratic model of the objective function at the current iterate x_k is

$$f(x_k + p) \approx m_k(p) = f_k + \nabla_k^T p + \frac{1}{2} p^T B_k p \tag{5.1}$$

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- The new iterate is

$$x_{k+1} = x_k + \alpha_k p_k \tag{5.3}$$

  where the step length α_k is chosen to satisfy the Wolfe conditions.

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- Suppose that we have generated a new iterate x_{k+1} and wish to construct a new quadratic model, of the form

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- What requirements should we impose on B_{k+1}? Based on the knowledge we have gained during the latest step.

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- We get

$$B_{k+1} s_k = y_k \tag{5.6}$$

which is referred as the *secant equation (割线方程)*

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  Sice $c_2 < 1$ and p_k is a decent direction, the right term is positive.

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- In other words, we solve the problem

$$\min_{B} \quad \|B - B_k\| \tag{5.8a}$$

$$s.t. \quad B = B^T, \quad Bs_k = y_k, \tag{5.8b}$$

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  where s_k and y_k satisfy the curvature condition (5.7) and B_k is symmetric and positive definite.
- Many matrix norms can be used in (5.8a), and each norm gives rise to a different quasi-Newton method.

The DFP Method

Theorem

Assume $B \in R^{n\times n}$ is symmetric, $c,\ s,\ y \in R^n$, satisfying $c^T s > 0$. Suppose $M \in R^{n\times n}$ is a nonsingular symmetric matrix, satisfying $c = M^{-2}s$, then

$$\bar{B} = B + \frac{(y - Bs)c^T + c(y - Bs)^T}{c^T s} - \frac{(y - Bs)^T s}{(c^T s)^2} cc^T$$

is the unique solution of the following minization problem

$$\min \left\{ \|\hat{B} - B\|_{M,F}, \quad s.t.\ \ \hat{B}s = y, \quad \hat{B}^T = \hat{B} \right\}$$

where $\|B\|_{M,F} = \|MBM\|_F$ and $\|\cdot\|_F$ is the Frobenius norm defined by $\|C\|_F = \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij}^2$

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$$\bar{B} - B = \frac{(y - Bs)c^T + c(y - Bs)^T}{c^T s} - \frac{(y - Bs)^T s}{(c^T s)^2} c c^T$$

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$$\bar{E} = \frac{E z z^T + z z^T E}{z^T z} - \frac{z^T E z}{(z^T z)^2} z z^T.$$

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- Moreover, if $v^T z = 0$, then $\|\bar{E}v\|_2 \leq \|Ev\|_2$.

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- Hence $\|\bar{E}\|_F \leq \|E\|_F$.

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- Hence $\|\bar{E}\|_F \leq \|E\|_F$.
- Moreover, $f(\hat{B}) = \|\hat{B} - B\|_{M,F}$ is strongly convex on the convex set $\{\hat{B} | \hat{B}s = y, \hat{B}^T = \hat{B}\}$, hence the solution $\hat{B}$ is the unique solution.

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Theorem Application

- In particular, let $c = y_k, \; B = B_k, \; s = s_k, \; y = y_k$ in above, we have the DFP formula

$$\begin{aligned} B_{k+1} &= B_k + \frac{(y_k - B_k s_k){y_k}^T + y_k(y_k - B_k s_k)^T}{{y_k}^T s_k} - \frac{(y_k - B_k s_k)^T s_k}{({y_k}^T s_k)^2} y_k {y_k}^T \\ &= B_k + \rho_k\big((y_k - B_k s_k){y_k}^T + y_k(y_k - B_k s_k)^T\big) + \rho_k^2 (y_k - B_k s_k)^T s_k y_k y \\ &= (I - \rho_k y_k s_k^T) B_k (I - \rho_k s_k y_k^T) + \rho_k y_k y_k^T \end{aligned}$$

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- Denote by $H_k = B_k^{-1}$. Utilizing Sherman-Morrison-Woodbury formula to derive

$$H_{k+1} = H_k - \frac{H_k y_k y_k H_k}{y_k^T H_k y_k} + \frac{s_k s_k^T}{y_k^T s_k}$$

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- $M =?$
- since $M^2 c = s$, $c = y_k$ and $s = s_k$ in DFP, hence $M^2 y_k = s_k$

The DFP Method

- One of Choices: $M^2 = \bar{G}_k^{-1}$ where $\bar{G}_k$ is the average Hessian defined by

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- With this weighting matrix and this norm, the unique solution of (5.8a) is

$$B_{k+1} = (I - \gamma_k y_k s_k^T) B_k (I - \gamma_k y_k s_k^T) + \gamma_k y_k y_k^T, \tag{5.9}$$

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- This formula is called the DFP updating formula, since it is the one originally proposed by Davidon in 1959, and subsequently studied, implemented, and popularized by Fletcher and Powell (1962).

The DFP Method

Properties

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Properties

- 对于二次目标函数 $f = \frac{1}{2}x^T Ax - b^T x$ (采用精确线搜索方法)

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  - 当采用精确线性搜索时，对于凸函数，方法具有全局收敛性。

THE DFP METHOD

Theorem (二次终止性定理)

如果 f是二次目标函数，A是其正定的Hessian矩阵，那么当采用精确线性搜索时， DFP方法具有遗传性质和方向共轭性质，即对于$i = 0, 1, \cdots, m$, 有

$$
\begin{aligned}
H_{i+1} y_j &= s_j, \quad j = 0, 1, \cdots, i \text{ 遗传性质} \\
s_i^T A s_j &= 0, \quad j = 0, 1, \cdots, i-1 \text{ 方向共轭性}
\end{aligned}
$$

方法在$m + 1 \le n$步迭代后终止。如果$m = n - 1$, 则$H_n = A^{-1}$。

The DFP Method

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\begin{aligned}
r_{i+1}^T s_j &= r_{j+1}^T s_j + \sum_{k=j+1}^{i} (r_{k+1}-r_k)^T s_j \\
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- 利用归纳假设 $H_{i+1}y_j = s_j$,, $As_j = A(x_{j+1}-x_j) = y_j$和上式,得到

$$
s_{i+1}^T A s_j = \alpha_{i+1} p_{i+1}^T A s_j = \alpha_{i+1}(-H_{i+1}r_{i+1})^T y_j = -\alpha_{i+1} g_{i+1}^T s_j = 0
$$

这就证明方向共轭性对于$i+1$也是成立的。

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Proof (Continue...)

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- 对于遗传性质，我们要证明$H_{i+2}y_j = s_j,\ j = 0, \cdots, i+1.$

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- 因此

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\begin{aligned}
H_{i+2}y_j &= H_{i+1}y_j + \frac{s_{i+1}s_{i+1}^T y_j}{s_{i+1}^T y_{i+1}} - \frac{H_{i+1}y_{i+1}y_{i+1}^T H_{i+1}y_j}{y_{i+1}^T H_{i+1} y_{i+1}} \\
&= H_{i+1}y_j = s_j
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这就证明了遗传性质对$i+1$也是成立的。

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- 当$m=n-1$时，由于s_i线性无关，$i=0,\cdots,n-1$，故 $H_n y_j = s_j$, $j=0,\cdots,n-1$, 此即 $H_n A s_j = s_j$, $j=0,\cdots,n-1$.

从而有$H_n = A^{-1}$。

The DFP Method

Theorem (DFP方法的正定性)

当且仅当$s_k^T y_k > 0$时，DFP的校正公式$H_{k+1} = H_k + \frac{s_k s_k^T}{s_k^T y_k} - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k}$保持正定性。

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- Infinite solutions of H_{k+1}.

BFGS Method

- The condition of closeness to H_k is now specified by

$$\min_{H} \quad \|H - H_k\|_{M,F} \tag{5.11}$$

$$s.t. \quad H = H^T, \quad H y_k = s_k. \tag{5.12}$$

- The norm is again the weighted Frobenius norm described above, where the weight matrix M^2 is now any matrix satisfying

$$M^2 s_k = y_k$$

- Assume again that M^2 is given by the average Hessian $\bar{G}_k$. The unique solution H_{k+1} to (5.11) is given by

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k s_k y_k^T) + \rho_k s_k s_k^T, \tag{5.13}$$

with $\rho_k = \frac{1}{y_k^T s_k}$.

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$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} \tag{5.14}$$

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- It is interesting to note that the DFP and BFGS updating formulae are duals of each other (互为对偶), in the sense that one can be obtained from the other by the interchanges $s \leftrightarrow y$, $B \leftrightarrow H$.

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End(while)

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- Though Newton's method converges more rapidly (that is quadratically), its cost per iteration is higher because it requires the solution of a linear system.
- A more important advantage for BFGS is, of course, that it does not require calculation of second derivatives.

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    - then the Hessian approximation will tend to correct itself within a few steps
    - The self correcting properties of BFGS hold only when an adequate line search is performed.
    - In particular, the Wolfe line search conditions ensure that the quadratic model to capture appropriate curvature information.

The BFGS Method - Implementation Details

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    - If β is "too large" so that the first step $p_0 = -\beta g_0$ is too long, many function evaluations may be required to find a suitable value for the step length α_0.
    - Some software asks the user to prescribe a value δ for the norm of the first step, and then set $H_0 = \delta \|g_0\|^{-1} I$ to achieve this norm.

The BFGS Method - Implementation

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- In BFGS, $M^2 = \bar{G}_k$ and $M^2 y_k = s_k$. Let $z_k = M^{-1} s_k$, 则$y_k = M^{-1} z_k$,

$$\frac{y_k^T s_k}{y_k^T y_k} = \frac{(M^{-1} z_k)^T M z_k}{z_k M^{-2} z_k} = \frac{z_k^T z_k}{z_k \bar{G}_k z_k}$$

The BFGS Method - Implementation

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- Computational observations strongly suggest that it is more economical, in terms of function evaluations, to perform a fairly inaccurate line search. The values $c_1 = 10^{-4}$ and $c_2 = 0.9$ are commonly used.
- The performance of the BFGS method can degrade if the line search is not based on the Wolfe conditions.

Numerical Experiment Results

Rosenbrock's function
$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

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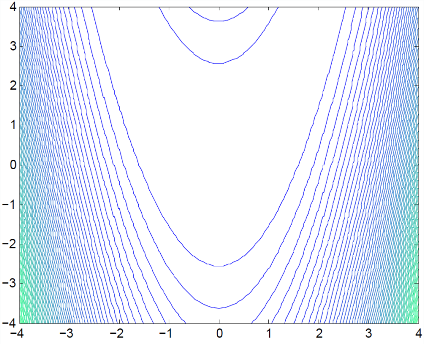

Numerical Experiment Results

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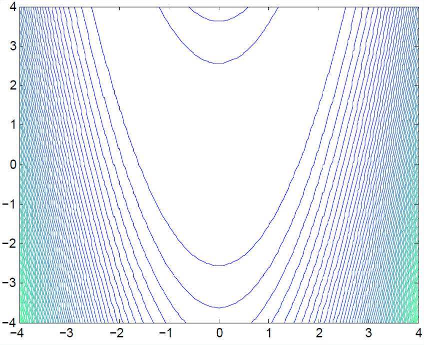
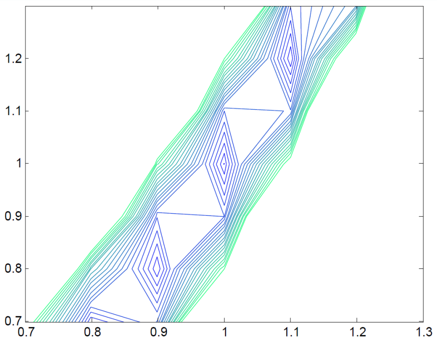
The optimal solution is $x^* = (1,1)^T$, $f(x^*) = 0$.





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- The initial point $x_0 = (-1.2, 1)$.
- The steepest descent method required 5264 iterations, whereas BFGS and Newton took only 34 and 21 iterations, respectively to reduce the gradient norm to 10^{-5}.

steepest descent	BFGS	Newton
1.827e-04	1.70e-03	3.48e-02
1.826e-04	1.17e-03	1.44e-02
1.824e-04	1.34e-04	1.82e-04
1.823e-04	1.01e-06	1.17e-08

The value of $\|x_k - x^*\|$ in last few iterations of the steepest descent, BFGS, and an inexact Newton method on Rosenbrock's function

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- Unlike the rank-two update formulae, this *symmetric-rank-1* , or SR1, update does not guarantee that the updated matrix maintains positive definiteness. Good numerical results have been obtained with algorithms based on SR1.

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- Thus, $v = \delta(y_k - B_k s_k)$ for some scalar δ.
- Substituting this form of v into the secant equation, we obtain

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- Therefore, we choose the parameters δ and σ to be

$$\sigma = \mathrm{sign}[s_k^T (y_k - B_k s_k)], \quad \delta = \pm [|s_k^T (y_k - B_k s_k)|]^{-\frac{1}{2}}.$$

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- SR1 method is self-dual, i.e. the inverse formula H_k can be obtained simply by replacing B, s and y by H, y and s, respectively.

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- However, with the advent of trust-region methods, the SR1 updating formula has proved to be quite useful.
- its ability to generate indefinite Hessian approximations can actually be regarded as one of its chief advantages.

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- If $y_k = B_k s_k$, then the only updating formula satisfying the secant equation is simply $B_{k+1} = B_k$;
- If $y_k \neq B_k s_k$ and $(y_k - B_k s_k)^T s_k = 0$, then there is no symmetric rank-one updating formula satisfying the secant equation.

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- It suggests that rank-one updating does not provide enough freedom to develop a matrix with all the desired characteristics, and that a rank-two correction is required.
- This reasoning leads us back to the BFGS method, in which positive definiteness (and thus nonsingularity) of all Hessian approximations is guaranteed.

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A strategy to prevent the SR1 method from breaking down

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- More specifically, the SR1 update is applied only if

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- Most implementations of the SR1 method use a skipping rule of this kind.

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- $s_k^T y_k \geq 0$ required for BFGS updating may easily fail if the line search does not impose the Wolfe conditions (e.g., if the step is not long enough).
- Therefore skipping the BFGS update can occur often and can degrade the quality of the Hessian approximation.

SR1 Properties

定理：二次终止性

Suppose that $f : R^n \to R$ is a strongly convex quadratic function $f(x) = b^T x + \frac{1}{2}x^T Ax$, where A is symmetric positive definite.
Then for any starting point x_0 and any symmetric starting matrix H_0, the iterates $\{x_k\}$ generated by the SR1 method converge to the minimizer in at most n steps, provided that $(s_k - H_k y_k)^T y_k \neq 0$ for all k. Moreover, if n steps are performed, and if the search directions p_k are linearly independent, then $H_n = A^{-1}$.

THE BROYDEN CLASS

The Broyden Class

- A family of updates specified by the following general formula

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} + \phi_k (s_k^T B_k s_k) v_k v_k^T \tag{5.18}$$

where ϕ_k is a scalar parameter and

$$v_k = \left(\frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k} \right).$$

The Broyden Class

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- The BFGS and DFP methods are members of the Broyden class-we recover BFGS by setting $\phi_k = 0$, DFP by setting $\phi_k = 1$, and SR1 by setting $\phi_k = \frac{s_k^T y_k}{(s_k - H_k y_k)^T y_k}$ in (5.18).

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- This relationship indicates that all members of the Broyden class satisfy the secant equation
- members with $0 \leq \phi_k \leq 1$(restricted Broyden class) preserve positive definiteness of the Hessian approximations when $s_k^T y_k > 0$.
(由于DFP方法保持正定性，当$\phi \geq 0$由联锁特征值定理可知，Broyden校正后的特征值不小于H_{k+1}^{DFP}的最小特征值, 可以得到保持正定性.)

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$$\phi_k^c = \frac{1}{1-\mu_k}, \text{ with } \mu_k = \frac{(y_k^T B_k^{-1} y_k)(s_k^T B_k s_k)}{(y_k^T s_k)^2}. \tag{5.20}$$

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- By applying the Cauchy-Schwarz inequality to (5.20) we see that $\mu_k \geq 1$ and therefore $\phi_k^c \leq 0$.
- Hence, if the initial Hessian approximation B_0 is symmetric and positive definite, and if $s_k^T y_k > 0$ and $\phi_k > \phi_k^c$ for each k, then all the matrices B_k generated by Broyden's formula (5.18) remain symmetric and positive definite.

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- When the line search is exact, all methods in the Broyden class with $\phi_k \geq \phi_k^c$ generate the same sequence of iterates (由于p_k与ϕ无关).
- This result applies to general nonlinear functions and is based on the observation that when all the line searches are exact, the directions generated by Broyden-class methods differ only in their lengths.
- The line searches identify the same minima along the chosen search direction, though the values of the line search parameter may differ because of the different scaling.

Properties of the Broyden Class

The Broyden class has several remarkable properties when applied with exact line searches to quadratic functions.

Theorem: 二次终止性、遗传性和共轭性

- Suppose that a method in the Broyden class is applied to a strongly convex quadratic function $f : \mathcal{R}^n \to \mathcal{R}$, where x_0 is the starting point and B_0 is any symmetric and positive definite matrix.
- Assume that α_k is the exact step length and the chosen value of ϕ_k did not produce a singular update matrix.
- Then the following statements are true:

Properties of the Broyden Class

Theorem(continue..)

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3. If the starting matrix is $B_0 = I$, then the iterates are identical to those generated by the conjugate gradient method. In particular, the search directions are conjugate, that is,

$$s_i^T A s_j = 0 \text{ for } i \neq j$$

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4. If the starting matrix B_0 is not the identity matrix, then the Broyden-class method is identical to the preconditioned conjugate gradient method that uses B_0 as preconditioner.
5. If n iterations are performed, we have $B_{n+1} = A$.

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- The results in the above theorem would appear to be mainly of theoretical interest,
- since the inexact line searches used in practical implementations of Broyden-class methods (and all other quasi-Newton methods) cause their performance to differ markedly.
- Nevertheless, this type of analysis guided most of the development of quasi-Newton methods.

CONVERGENCE ANALYSIS

- Although the BFGS and SR1 methods are known to be remarkably robust in practice, we will not be able to establish truly global convergence results for general nonlinear objective functions.
- That is, we cannot prove that the iterates of these quasi-Newton methods approach a stationary point of the problem from any starting point and any (suitable) initial Hessian approximation.
- In fact, it is not yet known if the algorithms enjoy such properties.
- In our analysis we will either assume that the objective function is convex or that the iterates satisfy certain properties.
- On the other hand, there are well known local, superlinear convergence results that are true under reasonable assumptions.

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- Let B_0 be any symmetric positive definite initial matrix, and let x_0 be a starting point for which
  1. the objective function f is twice continuously differentiable.
  2. level set $\mathcal{L} = \{x \in \mathcal{R}^n | f(x) \leq f(x_0)\}$ is convex
  3. there exist positive constants m and M such that

$$m\|z\|^2 \leq z^T \nabla^2 f(x) z \leq M\|z\|^2$$

- Then the sequence $\{x_k\}$ generated by Algorithm 1 converges to the minimizer x^* of f.

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- The above theorem has been generalized to the entire restricted Broyden class, except for the DFP method;
- An extension of the analysis shows that the rate of convergence of the iterates is linear.
- In particular, we can show that the sequence $\|x_k - x^*\|$ converges to zero rapidly enough that

$$\sum_{k=1}^{\infty} \|x_k - x^*\| < \infty. \tag{5.21}$$

Superlinear Convergence of BFGS

Theorem

- Suppose that f is twice continuously differentiable
- Hessian matrix $\nabla^2 f$ is Lipschitz continuous at x^* that is,

$$\|\nabla^2 f(x) - \nabla^2 f(x^*)\| \leq L\|x - x^*\|$$

  for all x near x^*, where L is a positive constant.
- Suppose (5.21) holds.

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- Suppose (5.21) holds.
- Then x_k converges to x^* at a superlinear rate.

Convergence of SR1 Method

Theorem

- Suppose that the iterates x_k are generated by Algorithm 2 . Suppose also that the following conditions hold:
  1. The sequence of iterates does not terminate, but remains in a closed, bounded, convex set $\mathcal{D}$, on which the function f is twice continuously differentiable, and in which f has a unique stationary point x^*;
  2. the Hessian $\nabla^2 f(x^*)$ is positive definite, and $\nabla^2 f(x)$ is Lipschitz continuous in a neighborhood of x^*;
  3. the sequence of matrices $\{B_k\}$ is bounded in norm;
  4. condition (5.17) holds at every iteration, where r is some constant in $(0, 1)$.
- Then

$$\lim_{k\to\infty} x_k = x^*, \text{ and } \lim_{k\to\infty} \frac{\|x_{k+n+1} - x^*\|}{\|x_k - x^*\|} = 0$$

Thanks For Your Attention