Line-Search Methods for Smooth Unconstrained Optimization

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Notes

Outline

Notes

The problem

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x)$$

where the objective function $f : \mathbb{R}^n \to \mathbb{R}$

- assume that $f \in \mathcal{C}^1$ (sometimes $\mathcal{C}^2$) and is Lipschitz continuous
- in practice this assumption may be violated, but the algorithms we develop may still work
- in practice it is very rare to be able to provide an explicit minimizer
- we consider iterative methods: given starting guess x_0, generate sequence

$$\{x_k\} \quad \text{for } k = 1, 2, \ldots$$

- AIM: ensure that (a subsequence) has some favorable limiting properties
  - satisfies first-order necessary conditions
  - satisfies second-order necessary conditions

Notation: $f_k = f(x_k), g_k = g(x_k), H_k = H(x_k)$

Notes

The basic idea

- consider descent methods, i.e., $f(x_{k+1}) < f(x_k)$
- calculate a search direction p_k from x_k
- ensure that this direction is a descent direction, i.e.,

$$g_k^T p_k < 0 \quad \text{if} \quad g_k \neq 0$$

  so that, for small steps along p_k, the objective function f **will** be reduced
- calculate a suitable steplength $\alpha_k > 0$ so that

$$f(x_k + \alpha_k p_k) < f_k$$

- computation of α_k is the linesearch
- the computation of α_k may itself require an iterative procedure
- generic update for linesearch methods is given by

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

Notes

Issue 1: steps might be too long

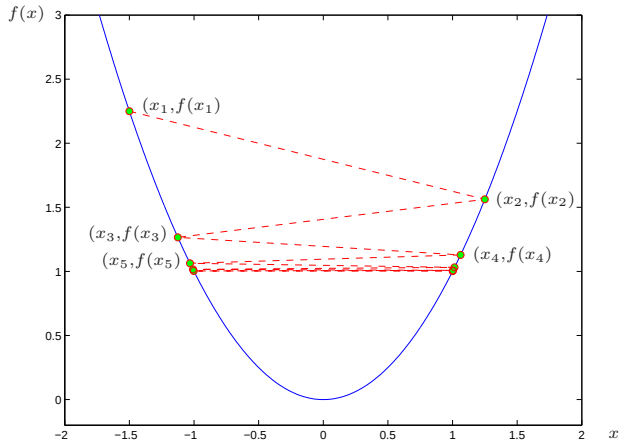

Figure: The objective function $f(x) = x^2$ and the iterates $x_{k+1} = x_k + \alpha_k p_k$ generated by the descent directions $p_k = (-1)^{k+1}$ and steps $\alpha_k = 2 + 3/2^{k+1}$ from $x_0 = 2$.

- decrease in f is not proportional to the size of the directional derivative!

Notes

Issue 2: steps might be too short

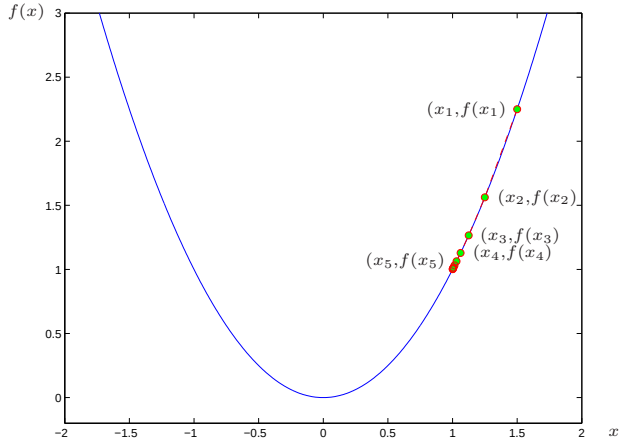

Figure: The objective function $f(x) = x^2$ and the iterates $x_{k+1} = x_k + \alpha_k p_k$ generated by the descent directions $p_k = -1$ and steps $\alpha_k = 1/2^{k+1}$ from $x_0 = 2$.

- decrease in f is not proportional to the size of the directional derivative!

Notes

What is a practical linesearch?

- in the "early" days exact linesearchs were used, i.e., pick α_k to minimize

$$f(x_k + \alpha p_k)$$

  - an exact linesearch requires univariate minimization
  - cheap if f is simple, e.g., a quadratic function
  - generally very expensive and not cost effective
  - exact linesearch may not be much better than an approximate linesearch

- modern methods use inexact linesearchs
  - ensure steps are neither too long nor too short
  - make sure that the decrease in f is proportional to the directional derivative
  - try to pick "appropriate" initial stepsize for fast convergence
    - ⋆ related to how the search direction s_k is computed

- the descent direction (search direction) is also important
  - "bad" directions may not converge at all
  - more typically, "bad" directions may converge very slowly

Notes

Definition 2.1 (Steepest descent direction)

For a differentiable function f, the search direction

$$p_k \stackrel{\text{def}}{=} -\nabla f(x_k) \equiv -g_k$$

is called the steepest-descent direction.

- p_k is a descent direction provided $g_k \neq 0$
  - $g_k^T p_k = -g_k^T g_k = -\|g_k\|_2^2 < 0$
- p_k solves the problem

$$\underset{p \in \mathbb{R}^n}{\text{minimize}} \;\; m_k^L(x_k + p) \;\; \text{subject to} \;\; \|p\|_2 = \|g_k\|_2$$

  - $m_k^L(x_k + p) \stackrel{\text{def}}{=} f_k + g_k^T p$
  - $m_k^L(x_k + p) \approx f(x_k + p)$

Any method that uses the steepest-descent direction is a method of steepest descent.

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Observation: the steepest descent direction is also the unique solution to

$$\underset{p \in \mathbb{R}^n}{\text{minimize}} \; f_k + g_k^T p + \tfrac{1}{2} p^T p$$

- approximates second-derivative Hessian by the identify matrix I
- how often is this a good idea?
- is it a surprise that convergence is typically very slow?

Idea: choose positive definite B_k and compute search direction as the unique minimizer

$$p_k = \underset{p \in \mathbb{R}^n}{\text{argmin}} \; m_k^Q(p) \stackrel{\text{def}}{=} f_k + g_k^T p + \tfrac{1}{2} p^T B_k p$$

- p_k satisfies $B_k p_k = -g_k$
- why must B_k be positive definite?
  - $B_k \succ 0 \implies M_k^Q$ is strictly convex $\implies$ unique solution
  - if $g_k \neq 0$, then $p_k \neq 0$ and is a descent direction

$$p_k^T g_k = -p_k^T B_k p_k < 0 \quad \implies \quad p_k \text{ is a descent direction}$$

- pick "intelligent" B_k that has "useful" curvature information
- IF $H_k \succ 0$ and we choose $B_k = H_k$, then s_k is the Newton direction. Awesome!

Notes

Question: How do we choose the positive-definite matrix B_k?

Ideally, B_k is chosen such that

- $\|B_k - H_k\|$ is "small"
- $B_k = H_k$ when H_k is "sufficiently" positive definite.

Comments:

- for the remainder of this section, we omit the suffix k and write $H = H_k$, $B = B_k$, and $g = g_k$.
- for a symmetric matrix $A \in \mathbb{R}^{n \times n}$, we use the matrix norm

$$\|A\|_2 = \max_{1 \leq j \leq n} |\lambda_j|$$

  with $\{\lambda_j\}$ the eigenvalues of A.
- the spectral decomposition of H is given by $H = V \Lambda V^T$, where

$$V = \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix} \quad \text{and} \quad \Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

  with $H v_j = \lambda_j v_j$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.
- H is positive definite if and only if $\lambda_j > 0$ for all j.
- computing the spectral decomposition is, generally, very expensive!

Notes

Method 1: small scale problems ($n < 1000$)

Algorithm 1 Compute modified Newton matrix B from H

1: **input** H
2: Choose $\beta > 1$, the desired bound on the condition number of B.
3: Compute the spectral decomposition $H = V\Lambda V^T$.
4: **if** $H = 0$ **then**
5: Set $\varepsilon = 1$
6: **else**
7: Set $\varepsilon = \|H\|_2/\beta > 0$
8: **end if**
9: Compute

$$\bar{\Lambda} = \mathbf{diag}(\bar{\lambda}_1, \bar{\lambda}_2, \ldots, \bar{\lambda}_n) \quad \text{with} \quad \bar{\lambda}_j = \begin{cases} \lambda_j & \text{if } \lambda_j \geq \varepsilon \\ \varepsilon & \text{otherwise} \end{cases}$$

10: **return** $B = V\bar{\Lambda}V^T \succ 0$, which satisfies $\mathbf{cond}(B) \leq \beta$

- replaces the eigenvalues of H that are "not positive enough" with ε
- $\bar{\Lambda} = \Lambda + D$, where

$$D = \mathbf{diag}\left(\max(0, \varepsilon - \lambda_1), \max(0, \varepsilon - \lambda_2), \ldots, \max(0, \varepsilon - \lambda_n)\right) \succeq 0$$

- $B = H + E$, where $E = VDV^T \succeq 0$

Notes

Question: What are the properties of the resulting search direction?

$$p = -B^{-1}g = -V\bar{\Lambda}^{-1}V^Tg = -\sum_{j=1}^{n} \frac{v_j^Tg}{\bar{\lambda}_j} v_j$$

Taking norms and using the orthogonality of V, gives

$$\begin{aligned} \|p\|_2^2 = \|B^{-1}g\|_2^2 &= \sum_{j=1}^{n} \frac{(v_j^Tg)^2}{\bar{\lambda}_j^2} \\ &= \sum_{\lambda_j \geq \varepsilon} \frac{(v_j^Tg)^2}{\lambda_j^2} + \sum_{\lambda_j < \varepsilon} \frac{(v_j^Tg)^2}{\varepsilon^2} \end{aligned}$$

Thus, we conclude that

$$\|p\|_2 = O\left(\frac{1}{\varepsilon}\right) \quad \text{provided } v_j^Tg \neq 0 \text{ for at least one } \lambda_j < \varepsilon$$

- the step p goes unbounded as $\varepsilon \to 0$ provided $v_j^Tg \neq 0$ for at least one $\lambda_j < \varepsilon$
- any indefinite matrix will generally satisfy this property
- the next method that we discuss is better!

Notes

Method 2: small scale problems ($n < 1000$)

Algorithm 2 Compute modified Newton matrix B from H

1: **input** H
2: Choose $\beta > 1$, the desired bound on the condition number of B.
3: Compute the spectral decomposition $H = V\Lambda V^T$.
4: **if** $H = 0$ **then**
5: Set $\varepsilon = 1$
6: **else**
7: Set $\varepsilon = \|H\|_2/\beta > 0$
8: **end if**
9: Compute

$$\bar{\Lambda} = \mathbf{diag}(\bar{\lambda}_1, \bar{\lambda}_2, \ldots, \bar{\lambda}_n) \quad \text{with} \quad \bar{\lambda}_j = \begin{cases} \lambda_j & \text{if } \lambda_j \geq \varepsilon \\ -\lambda_j & \text{if } \lambda_j \leq -\varepsilon \\ \varepsilon & \text{otherwise} \end{cases}$$

10: **return** $B = V\bar{\Lambda}V^T \succ 0$, which satisfies $\mathbf{cond}(B) \leq \beta$

- replace small eigenvalues λ_i of H with ε
- replace "sufficiently negative" eigenvalues λ_i of H with $-\lambda_i$
- $\bar{\Lambda} = \Lambda + D$, where

$$D = \mathbf{diag}\left(\max(0, -2\lambda_1, \varepsilon - \lambda_1), \ldots, \max(0, -2\lambda_n, \varepsilon - \lambda_n)\right) \succeq 0$$

- $B = H + E$, where $E = VDV^T \succeq 0$

Notes

Suppose that $B = H + E$ is computed from Algorithm 2 so that

$$E = B - H = V(\bar{\Lambda} - \Lambda)V^T$$

and since V is orthogonal that

$$\|E\|_2 = \|V(\bar{\Lambda} - \Lambda)V^T\|_2 = \|\bar{\Lambda} - \Lambda\|_2 = \max_j |\bar{\lambda}_j - \lambda_j|$$

By definition

$$\bar{\lambda}_j - \lambda_j = \begin{cases} 0 & \text{if} \quad \lambda_j \geq \varepsilon \\ \varepsilon - \lambda_j & \text{if } -\varepsilon < \lambda_j < \varepsilon \\ -2\lambda_j & \text{if} \quad \lambda_j \leq -\varepsilon \end{cases}$$

which implies that

$$\|E\|_2 = \max_{1 \leq j \leq n} \ \{\, 0,\ \varepsilon - \lambda_j,\ -2\lambda_j \,\}.$$

However, since $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, we know that

$$\|E\|_2 = \max \ \{\, 0,\ \varepsilon - \lambda_n,\ -2\lambda_n \,\}$$

- if $\lambda_n \geq \varepsilon$, i.e., H is sufficiently positive definite, then $E = 0$ and $B = H$
- if $\lambda_n < \varepsilon$, then $B \neq H$ and it can be shown that $\|E\|_2 \leq 2\max(\varepsilon, |\lambda_n|)$
- regardless, B is well-conditioned by construction

Notes

Example 2.2

Consider

$$g = \begin{pmatrix} 2 \\ 4 \end{pmatrix} \quad \text{and} \quad H = \begin{pmatrix} 1 & 0 \\ 0 & -2 \end{pmatrix}$$

- The Newton direction is

$$p^N = -H^{-1}g = \begin{pmatrix} -2 \\ 2 \end{pmatrix} \quad \text{so that} \quad g^T p^N = 4 > 0 \quad \text{(ascent direction)}$$

  and p^N is a saddle point of the quadratic model $g^T p + \frac{1}{2} p^T H p$ since H is indefinite.
- Algorithm 1 (Method 1) generates

$$B = \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}$$

  so that

$$p = -B^{-1}g = \begin{pmatrix} -2 \\ -\frac{4}{\varepsilon} \end{pmatrix} \quad \text{and} \quad g^T p = -4 - \frac{16}{\varepsilon} < 0 \quad \text{(descent direction)}$$

- Algorithm 2 (Method 2) generates

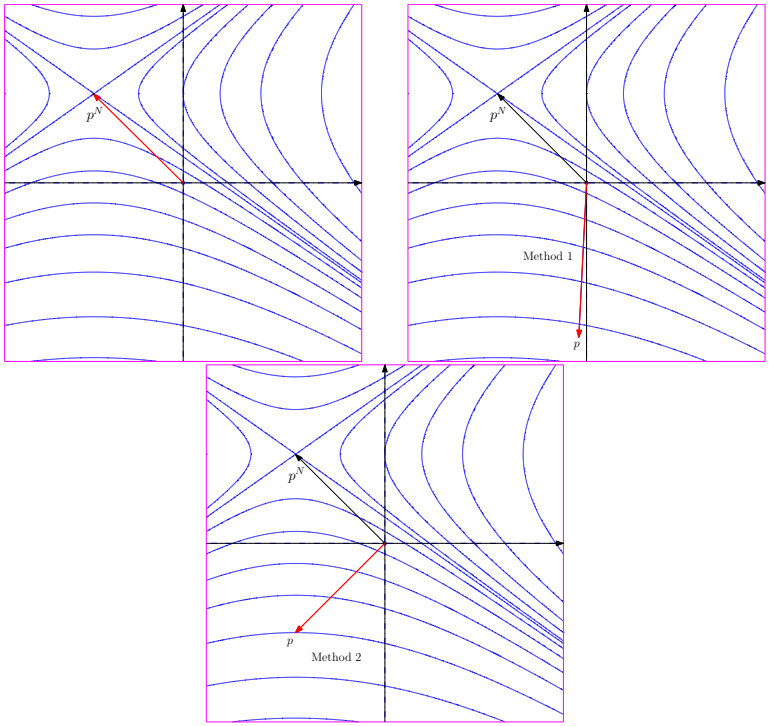
$$B = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

  so that

$$p = -B^{-1}g = \begin{pmatrix} -2 \\ -2 \end{pmatrix} \quad \text{and} \quad g^T p = -12 < 0 \quad \text{(descent direction)}$$

Notes

Notes



Question: What is the geometric interpretation?

Answer: Let the spectral decomposition of H be

$$H = V \Lambda V^T$$

and assume that $\lambda_j \neq 0$ for all j. Partition the eigenvector and eigenvalue matrices as

$$\Lambda = \begin{pmatrix} \Lambda_+ & \\ & \Lambda_- \end{pmatrix} \begin{matrix} \} \lambda_j > 0 \\ \} \lambda_j < 0 \end{matrix} \quad \text{and} \quad V = \begin{pmatrix} \underbrace{V_+}_{\lambda_j > 0} & \underbrace{V_-}_{\lambda_j < 0} \end{pmatrix}$$

So that $H = \begin{pmatrix} V_+ & V_- \end{pmatrix} \begin{pmatrix} \Lambda_+ & \\ & \Lambda_- \end{pmatrix} \begin{pmatrix} V_+^T \\ V_-^T \end{pmatrix}$ and the Newton direction is

$$\begin{aligned} p^N &= -V\Lambda^{-1}V^T g = -\begin{pmatrix} V_+ & V_- \end{pmatrix} \begin{pmatrix} \Lambda_+^{-1} & \\ & \Lambda_-^{-1} \end{pmatrix} \begin{pmatrix} V_+^T \\ V_-^T \end{pmatrix} g \\ &= -\begin{pmatrix} V_+ & V_- \end{pmatrix} \begin{pmatrix} \Lambda_+^{-1} & \\ & \Lambda_-^{-1} \end{pmatrix} \begin{pmatrix} V_+^T g \\ V_-^T g \end{pmatrix} \\ &= -V_+\Lambda_+^{-1}V_+^T g - V_-\Lambda_-^{-1}V_-^T g \\ &= \underbrace{-V_+\Lambda_+^{-1}V_+^T g}_{p_+^N} \quad \underbrace{-V_-\Lambda_-^{-1}V_-^T g}_{p_-^N} \stackrel{\text{def}}{=} p_+^N + p_-^N \end{aligned}$$

where

$$p_+^N = -V_+\Lambda_+^{-1}V_+^T g \quad \text{and} \quad p_-^N = -V_-\Lambda_-^{-1}V_-^T g$$

Notes

Result

Given $m_k^Q(p) = g^T p + \frac{1}{2} p^T H p$ with H nonsingular, the Newton direction

$$p^N = p_+^N + p_-^N = -V_+\Lambda_+^{-1}V_+^T g - V_-\Lambda_-^{-1}V_-^T g$$

is such that

- p_+^N minimizes $m_k^Q(p)$ on the subspace spanned by V_+.
- p_-^N maximizes $m_k^Q(p)$ on the subspace spanned by V_-.

Notes

Proof:

- The function $\psi(y) \stackrel{\text{def}}{=} m_k^Q(V_+ y)$ may be written as

$$\psi(y) = g^T V_+ y + \tfrac{1}{2} y^T V_+^T H V_+ y$$

and has a stationary point y^* given by

$$y^* = -(V_+^T H V_+)^{-1} V_+^T g$$

Since

$$\nabla^2 \psi(y) = V_+^T H V_+ = V_+^T V \Lambda V^T V_+ = \Lambda_+ \succ 0$$

we know that y^* is, in fact, the unique minimizer of $\psi(y)$ and

$$V_+ y^* = -V_+ \Lambda_+^{-1} V_+^T g \equiv p_+^N$$

- For the second part

$$y^* = -(V_-^T H V_-)^{-1} V_-^T g = -\Lambda_-^{-1} V_-^T g$$

so that

$$V_- y^* = -V_- \Lambda_-^{-1} V_-^T g \equiv p_-^N.$$

Since $\Lambda_- \prec 0$, we know that p_-^N maximizes $m_k^Q(p)$ on the space spanned by the columns of V_-. ∎

Notes

Some observations

- p_+^N is a descent direction for f:

$$g^T p_+^N = -g^T V_+ \Lambda_+^{-1} V_+^T g = -y^T \Lambda_+^{-1} y \leq 0$$

where $y \stackrel{\text{def}}{=} V_+^T g$. The inequality is strict if $y \neq 0$, i.e., g is not orthogonal to the column space of V_+

- p_-^N is an ascent direction for f:

$$g^T p_-^N = -g^T V_- \Lambda_-^{-1} V_-^T g = -y^T \Lambda_-^{-1} y \geq 0$$

where $y \stackrel{\text{def}}{=} V_-^T g$. The inequality is strict if $y \neq 0$, i.e., g is not orthogonal to the column space of V_-

- $p^N = p_+^N + p_-^N$ may or may not be a descent direction!
- This is the geometry of the Newton direction. What about the modified Newton direction?

Notes

Question: what is the geometry of the modifed-Newton step?
Answer: Partition the matrices in the spectral decomposition $H = V\Lambda V^T$ such that

$$V = [V_+ \;\; V_\varepsilon \;\; V_-] \quad \text{and} \quad \Lambda = \begin{pmatrix} \Lambda_+ & & \\ & \Lambda_\varepsilon & \\ & & \Lambda_- \end{pmatrix}$$

where

$$\Lambda_+ = \{\lambda_i : \lambda_i \geq \varepsilon\} \qquad \Lambda_\varepsilon = \{\lambda_i : |\lambda_i| < \varepsilon\} \qquad \Lambda_- = \{\lambda_i : \lambda_i \leq -\varepsilon\}$$

Theorem 2.3 (Properties of the modifed-Newton direction)

Suppose that the positive-definite matrix B_k is computed from Algorithm 2 with input H_k and value $\varepsilon > 0$. If $g_k \neq 0$ and p_k is the unique solution to $B_k p = -g_k$, then p_k may be written as $p_k = p_+ + p_\varepsilon + p_-$, where

(i) *p_+ is a direction of positive curvature that minimizes $m_k^Q(p)$ in the space spanned by the columns of V_+;*

(ii) *$-(p_-)$ is a direction of negative curvature that maximizes $m_k^Q(p)$ in the space spanned by the columns of V_-; and*

(iii) *p_ε is a multiple of the steepest-descent direction in the space spanned by the columns of V_ε with $\|p_\varepsilon\|_2 = O(1/\varepsilon)$.*

Comments:

- implies that singular Hessians H_k may easily cause numerical difficulties
- the direction p_- is the negative of p_-^N associated with the Newton step

Notes

Main goals of quasi-Newton methods

- Maintain positive-definite "approximation" B_k to H_k
- Instead of computing B_{k+1} from scratch, e.g., from a spectral decomposition of H_{k+1}, want to compute B_{k+1} as an update to B_k using information at x_{k+1}
- inject "real" curvature information from $H(x_{k+1})$ into B_{k+1}
- Should be cheap to form and compute with B_k
- be applicable for medium-scale problems ($n \approx 1000 - 10,000$)
- Hope that fast convergence (superlinear) of the iterates $\{x_k\}$ computed using B_k can be recovered

Notes

The optimization problem solved in the $(k+1)$st iterate will be

$$\underset{p\in\mathbb{R}^n}{\text{minimize}} \;\; m_{k+1}^Q(p) \stackrel{\text{def}}{=} f_{k+1} + g_{k+1}^T p + \tfrac{1}{2} p^T B_{k+1} p$$

How do we choose B_{k+1}?

How about to satisfy the following:

- the model should agree with f at x_{k+1}
- the gradient of the model should agree with the gradient of f at x_{k+1}
- the gradient of the model should agree with the gradient of f at x_k (previous point)

These are equivalent to

1. $m_{k+1}^Q(0) = f_{k+1}$ ✓ already satisfied
2. $\nabla m_{k+1}^Q(0) = g_{k+1}$ ✓ already satisfied
3. $\nabla m_{k+1}^Q(-\alpha_k p_k) = g_k$

$$B_{k+1}(-\alpha_k p_k) + g_{k+1} = g_k \quad \Longleftrightarrow \quad B_{k+1}\underbrace{(x_{k+1} - x_k)}_{s_k} = \underbrace{g_{k+1} - g_k}_{y_k}$$

Thus, we aim to cheaply compute a symmetric positive-definite matrix B_{k+1} that satisfies the so-called secant equation

$$B_{k+1}s_k = y_k \quad \text{where } s_k \stackrel{\text{def}}{=} x_{k+1} - x_k \text{ and } y_k \stackrel{\text{def}}{=} g_{k+1} - g_k$$

Notes

Observation: If the matrix B_{k+1} is positive definite, then the curvature condition

$$s_k^T y_k > 0 \tag{1}$$

is satisfied.

- using the fact that $B_{k+1}s_k = y_k$, we see that

  $$s_k^T y_k = s_k^T B_{k+1} s_k$$

  which must be positive if $B_{k+1} \succ 0$
- the previous relation explains why (1) is called a curvature condition
- (1) will hold for any two points x_k and x_{k+1} if f is strictly convex
- (1) does not always hold for any two points x_k and x_{k+1} if f is nonconvex
- for nonconvex functions, we need to be careful how we choose α_k that defines $x_{k+1} = x_k + \alpha_k p_k$ (see Wolfe conditions for linesearch strategies)

Note: for the remainder, I will drop the subscript k from all terms.

Notes

The problem

Given a symmetric positive-definite matrix B, and vectors s and y, find a symmetric positive-definite matrix $\bar{B}$ that satisfies the secant equation

$$\bar{B}s = y$$

Want a cheap update, so let us first consider a rank-one update of the form

$$\bar{B} = B + uv^T$$

for some vectors u and v that we seek.

Derivation:

Case 1: $Bs = y$
Choose $u = v = 0$ since

$$\bar{B}s = (B + uv^T)s = Bs + uv^Ts = y$$

Case 2: $Bs \neq y$
If $u = 0$ or $v = 0$ then

$$\bar{B}s = (B + uv^T)s = Bs + uv^Ts = Bs \neq y$$

So search for $u \neq 0$ and $v \neq 0$. Symmetry of B and desired symmetry of $\bar{B}$ imply that

$$\bar{B} = \bar{B}^T \iff B + uv^T = B^T + vu^T \iff uv^T = vu^T$$

But $uv^T = vu^T$, $u \neq 0$, and $v \neq 0$ imply that $v = \alpha u$ for some $\alpha \neq 0$ (exercise). Thus, we should search for an $\alpha \neq 0$ and $u \neq 0$ such that the secant condition is satisfied by

$$\bar{B} = B + \alpha uu^T$$

Notes

From previous slide, we hope to find an $\alpha > 0$ and $u \neq 0$ so that

$$\bar{B} = B + \alpha uu^T$$

satisfies

$$y \overset{\text{want}}{=} \bar{B}s = Bs + \alpha uu^Ts = Bs + \alpha(u^Ts)u$$

which implies

$$\alpha(u^Ts)u = y - Bs \neq 0.$$

This implies that

$$u = \beta(y - Bs) \quad \text{for some } \beta \neq 0.$$

Plugging back in, we are searching for

$$\begin{aligned}\bar{B} &= B + \alpha\beta^2(y - Bs)(y - Bs)^T \\ &= B + \gamma(y - Bs)(y - Bs)^T \quad \text{for some } \gamma \neq 0\end{aligned}$$

that satisfies the secant equation

$$y \overset{\text{want}}{=} \bar{B}s = Bs + \gamma(y - Bs)^Ts(y - Bs)$$

which implies

$$y - Bs = \gamma(y - Bs)^Ts(y - Bs)$$

which means we can choose

$$\gamma = \frac{1}{(y - Bs)^Ts} \quad \text{provided } (y - Bs)^Ts \neq 0.$$

Notes

Definition 2.4 (SR1 quasi-Newton formula)

If $(y - Bs)^T s \neq 0$ for some symmetric matrix B and vectors s and y, then the symmetric rank-1 (SR1) quasi-Newton formula for updating B is

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

and satisfies

- $\bar{B}$ is symmetric
- $\bar{B}s = y$ (secant condition)

In practice, we choose some $\kappa \in (0, 1)$ and then use

$$\bar{B} = \begin{cases} B + \frac{(y-Bs)(y-Bs)^T}{(y-Bs)^T s} & \text{if } |s^T(y - Bs)| > \kappa \|s\|_2 \|y - Bs\|_2 \\ B & \text{otherwise} \end{cases}$$

to avoid numerical error.

Question: Is $\bar{B}$ positive definite if B is positive definite?
Answer: Sometimes....but sometimes not!

Notes

Example 2.5 (SR1 update is not necessarily positive definite)

Consider the SR1 update with

$$B = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \quad s = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \quad \text{and} \quad y = \begin{pmatrix} -3 \\ 2 \end{pmatrix}$$

The matrix B is positive definite with eigenvalues $\approx \{0.38, 2.6\}$. Moreover,

$$y^T s = \begin{pmatrix} -3 & 2 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \end{pmatrix} = 1 > 0$$

so that the necessary condition for $\bar{B}$ to be positive definite holds. The SR1 update gives

$$y - Bs = \begin{pmatrix} -3 \\ 2 \end{pmatrix} - \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 4 \end{pmatrix}$$

$$(y - Bs)^T s = \begin{pmatrix} 0 & 4 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \end{pmatrix} = -4$$

$$\bar{B} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{(-4)} \begin{pmatrix} 0 \\ 4 \end{pmatrix} \begin{pmatrix} 0 & 4 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & -3 \end{pmatrix}$$

The matrix $\bar{B}$ is indefinite with eigenvalues $\approx \{2.19, -3.19\}$.

Notes

Theorem 2.6 (convergence of SR1 update)

Suppose that

- f *is* $\mathcal{C}^2$ *on* $\mathbb{R}^n$
- $\lim_{k\to\infty} x_k = x^*$ *for some vector* x^*
- $\nabla^2 f$ *is bounded and Lipschitz continous in a neighborhood of* x^*
- *the steps* s_k *are uniformly linearly independent*
- $|s_k^T(y_k - B_k s_k)| > \kappa \|s_k\|_2 \|y_k - B_k s_k\|_2$ *for some* $\kappa \in (0,1)$

Then, the matrices generated by the SR1 formula satisfy

$$\lim_{k\to\infty} B_k = \nabla^2 f(x^*)$$

Comment: the SR1 updates may converge to an indefinite matrix

Notes

Some comments

- if B is symmetric, then the SR1 update $\bar{B}$ (when it exists) is symmetric
- if B is positive definite, then the SR1 update $\bar{B}$ (when it exists) is not necessarily positive definite
- linesearch methods require positive-definite matrices
- SR1 updating is not appropriate (in general) for linesearch methods
- SR1 updating is an attractive option for optimization methods that effectively utilize indefinite matrices (e.g., trust-region methods)
- to derive an updating strategy that produces positive-definite matrices, we have to look beyond rank-one updates. Would a rank-two update work?

Notes

For hereditary positive definiteness we must consider updates of at least rank two.

Result

U is a symmetric matrix of rank two if and only if

$$U = \beta uu^T + \delta ww^T,$$

for some nonzero β and δ, with u and w linearly independent.

If

$$\bar{B} = B + U$$

for some rank-two matrix U and $\bar{B}s = y$ for some vectors s and y, then

$$\bar{B}s = (B + U)s = y,$$

and it follows that

$$y - Bs = Us = \beta(u^T s)u + \delta(w^T s)w$$

Notes

Let us make the "obvious" choices of

$$u = Bs \quad \text{and} \quad w = y$$

which gives the rank-two update

$$U = \beta Bs(Bs)^T + \delta yy^T$$

and we now search for β and δ so that $\bar{B}s = y$ is satisfied. Substituting, we have

$$\begin{aligned} y \overset{\text{want}}{=} \bar{B}s &= (B + \beta Bs(Bs)^T + \delta yy^T)s \\ &= Bs + \beta Bss^T Bs + \delta yy^T s \\ &= Bs + \beta(s^T Bs)Bs + \delta(y^T s)y \end{aligned}$$

Making the "simple" choice of

$$\beta = -\frac{1}{s^T Bs} \quad \text{and} \quad \delta = \frac{1}{y^T s}$$

gives

$$\begin{aligned} \bar{B}s &= Bs - \frac{1}{s^T Bs}(s^T Bs)Bs + \frac{1}{y^T s}(y^T s)y \\ &= Bs - Bs + y = y \end{aligned}$$

as desired. This gives the Broyden, Fletcher, Goldfarb, Shanno (BFGS) quasi-Newton update formula.

Notes

Broyden, Fletcher, Goldfarb, Shanno (BFGS) update

Given a symmetric positive-definite matrix B and vectors s and y that satisfy $y^T s > 0$, the quasi-Newton BFGS update formula is given by

$$\bar{B} = B - \frac{1}{s^T B s} B s (B s)^T + \frac{1}{y^T s} y y^T \tag{2}$$

Result

If B is positive definite and $y^T s > 0$, then

$$\bar{B} = B - \frac{1}{s^T B s} B s (B s)^T + \frac{1}{y^T s} y y^T$$

is positive definite and satisfies $\bar{B} s = y$.

Proof:
Homework assignment. (hint: see the next slide)

Notes

A second derivation of the BFGS formula

Let $M = B^{-1}$ for some given symmetric positive definite matrix B. Solve

$$\underset{\bar{M} \in \mathbb{R}^{n \times n}}{\text{minimize}} \ \|\bar{M} - M\|_W \quad \text{subject to} \quad \bar{M} = \bar{M}^T, \quad \bar{M} y = s$$

for a "closest" symmetric matrix $\bar{M}$, where

$$\|A\|_W = \|W^{1/2} A W^{1/2}\|_F \quad \text{and} \quad \|C\|_F = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij}^2$$

for any weighting matrix W that satisfies $W y = s$. If we choose

$$W = G^{-1} \quad \text{and} \quad G = \int_0^1 [\nabla^2 f(y + \tau s)]^{-1} \, d\tau$$

then the solution is

$$\bar{M} = \left(I - \frac{s y^T}{y^T s} \right) M \left(I - \frac{y s^T}{y^T s} \right) + \frac{s s^T}{y^T s}.$$

Computing the inverse $\bar{B} = \bar{M}^{-1}$ using the Sherman-Morrison-Woodbury formula gives

$$\bar{B} = B - \frac{1}{s^T B s} B s (B s)^T + \frac{1}{y^T s} y y^T \quad \text{(BFGS formula again)}$$

so that $\bar{B} \succ 0$ if and only if $\bar{M} \succ 0$.

Notes

Recall: given the positive-definite matrix B and vectors s and y satisfying $s^T y > 0$, the BFGS formula (2) may be written as

$$\bar{B} = B - aa^T + bb^T$$

where

$$a = \frac{Bs}{(s^T Bs)^{1/2}} \quad \text{and} \quad b = \frac{y}{(y^T s)^{1/2}}$$

Limited-memory BFGS update

Suppose at iteration k we have m previous pairs (s_i, y_i) for $i = k-m, \ldots, k-1$. Then the limited-memory BFGS (L-BFGS) update with memory m and positive-definite seed matrix B_k^0 may be written in the form

$$B_k = B_k^0 + \sum_{i=k-m}^{k-1} \left[b_i b_i^T - a_i a_i^T \right]$$

for some vectors a_i and b_i that may be recovered via an unrolling formula (next slide).

- the positive-definite seed matrix B_k^0 is often chosen to be diagonal
- essentially perform m BFGS updates to the seed matrix B_k^0
- A different seed matrix may be used for each iteration k
  - Added flexibility allows "better" seed matrices to be used as iterations proceed

Notes

Algorithm 3 Unrolling the L-BFGS formula

1: **input** $m \geq 1$, $\{(s_i, y_i)\}$ for $i = k-m, \ldots, k-1$, and $B_k^0 \succ 0$
2: **for** $i = k-m, \ldots, k-1$ **do**
3: $\quad b_i \leftarrow y_i / (y_i^T s_i)^{1/2}$
4: $\quad a_i \leftarrow B_k^0 s_i + \sum_{j=k-m}^{i-1} \left[(b_j^T s_i) b_j - (a_j^T s_i) a_j \right]$
5: $\quad a_i \leftarrow a_i / (s_i^T a_i)^{1/2}$
6: **end for**

- typically $3 \leq m \leq 30$
- b_i and $b_j^T s_i$ should be saved and reused from previous iterations (exceptions are b_{k-1} and $b_j^T s_{k-1}$ because they depend on the most recent data obtained).
- with the previous savings in computation and assuming $B_k^0 = I$, the total cost to get the a_i, b_i vectors is approximately $\frac{3}{2} m^2 n$.
- cost of a matrix-vector product with B_k requires $4mn$ multiplications.
- other so-called compact representations are slightly more efficient

Notes

The problem of interest

Given a symmetric positive-definite matrix A, solve the linear system

$$Ax = b$$

which is equivalent to finding the unique minimizer of

$$\underset{x \in \mathbb{R}^n}{\text{minimize}}\ q(x) \stackrel{\text{def}}{=} \tfrac{1}{2} x^T A x - b^T x \tag{3}$$

because $\nabla q(x) = Ax - b$ and $\nabla^2 q(x) = A \succ 0$ implies that

$$\nabla q(x) = Ax - b = 0 \quad \Longleftrightarrow \quad Ax = b$$

- We seek a method that cheaply computes approximate solutions to the system $Ax = b$, or equivalent approximately minimizes (3).
- Do not want to compute a factorization of A, because it is assumed to be too expensive. We are interested in very large-scale problems
- We allow ourselves to compute matrix-vector products, i.e., Av for any vector v
- Why do we care about this? We will see soon!

Notation: $r(x) \stackrel{\text{def}}{=} Ax - b$ and $r_k \stackrel{\text{def}}{=} Ax_k - b$.

Notes

$$q(x) = \tfrac{1}{2} x^T A x - b^T x$$

Algorithm 4 Coordinate descent algorithm for minimizing q

input initial guess $x_0 \in \mathbb{R}^n$ and a symmetric positive-definite matrix $A \in \mathbb{R}^{n \times n}$
loop
  for $i = 0, 1, \ldots, n-1$ **do**
    Compute α_i as the solution to

$$\underset{\alpha \in \mathbb{R}}{\text{minimize}}\ q(x_i + \alpha e_{i+1}) \tag{4}$$

    $x_{i+1} \leftarrow x_i + \alpha_i e_{i+1}$
  end for
  $x_0 \leftarrow x_n$
end loop

- e_j represents the jth coordinate vector, i.e.,

$$e_j = (\ 0 \quad 0 \ \ldots \overbrace{1}^{j\text{th}} \ldots \ 0 \quad 0\ )^T \in \mathbb{R}^n$$

- Is it easy to solve (4)? Yes! (exercise)
- Does this work?

Notes

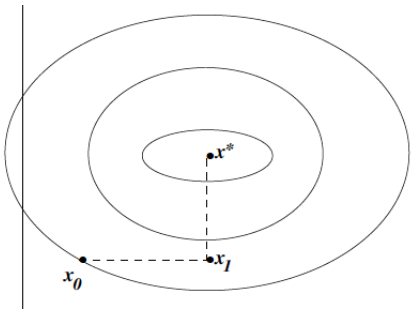


Figure: Coordinate descent converges in n steps. Very good! Axes are aligned with the coordinate directions e_i.

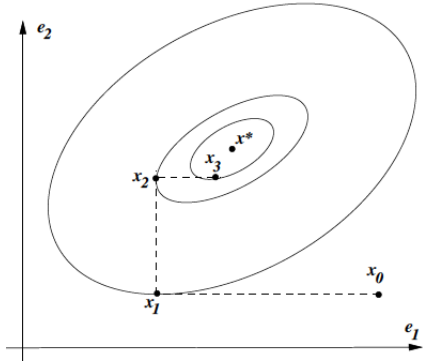


Figure: Coordinate descent does not converge in n steps. Looks like it will be very slow! Axes are not aligned with the coordinate directions e_i.

Fact: the axes are determined by the eigenvectors of A.

Observation: coordinate descent converges in no more than n steps if the eigenvectors align with the coordinate directions, i.e., $V = I$ where V is the eigenvector matrix of A.

Implication: Using the spectral decomposition of A

$$A = V\Lambda V^T = I\Lambda I^T = \Lambda \qquad \text{(a diagonal matrix)}$$

Conclusion: Coordinate descent converges in $\leq n$ steps when A is diagonal.

Notes

First thought: This is only good for diagonal matrices. That sucks!

Second thought: Can we use a transformation of variables so that the transformed Hessian is diagonal?

- Let S be a square nonsingular matrix and define the transformed variables

$$y = S^{-1}x \quad \Longleftrightarrow \quad Sy = x.$$

Consider the transformed quadratic function $\widehat{q}$ defined as

$$\widehat{q}(y) \stackrel{\text{def}}{=} q(Sy) \equiv \tfrac{1}{2}y^T \underbrace{S^TAS}_{\widehat{A}} y - (\underbrace{S^Tb}_{\widehat{b}})^T y = \tfrac{1}{2}y^T \widehat{A}y - \widehat{b}^T y$$

so that a minimizer x^* of q satisfies $x^* = Sy^*$ where y^* is a minimizer of $\widehat{q}$.

- If $\widehat{A} = S^TAS$ is diagonal, then applying the coordinate descent Algorithm 4 to $\widehat{q}$ would converge to y^* in $\leq n$ steps.
- $\widehat{A}$ is diagonal if and only if

$$s_i^TAs_j = 0 \quad \text{for all } i \neq j,$$

where

$$S = \begin{pmatrix} s_0 & s_1 & \dots & s_{n-1} \end{pmatrix}$$

- Line 5 of Algorithm 4 (in the transformed variables) is

$$y_{i+1} = y_i + \alpha_i e_{i+1}.$$

Multiplying by S and using $Sy = x$ leads to

$$x_{i+1} = Sy_{i+1} = S(y_i + \alpha_i e_{i+1}) = Sy_i + \alpha_i Se_{i+1} = x_i + \alpha_i s_i$$

Notes

Definition 2.7 (A-conjugate directions)

A set of nonzero vectors $\{s_0, s_1, \ldots, s_l\}$ is said to be conjugate with respect to the symmetric positive-definite matrix A (A-conjugate for short) if

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

- We want to find A-conjugate vectors.
- The eigenvectors of A are A-conjugate since the spectral decomposition gives

$$A = V \Lambda V^T \quad \Longleftrightarrow \quad V^T A V = \Lambda \quad \text{(diagonal matrix of eigenvalues)}$$

- Computing the spectral decomposition is too expensive for large scale problems.
- We want to find A-conjugate vectors cheaply!
- Let us look at a general algorithm.

Notes

Algorithm 5 General A-conjugate direction algorithm

1: **input** symmetric positive-definite matrix $A \in \mathbb{R}^{n \times n}$, and vectors x_0 and $b \in \mathbb{R}^n$.
2: Set $r_0 \leftarrow Ax_0 - b$ and $k \leftarrow 0$.
3: Choose direction s_0.
4: **while** $r_k \neq 0$ **do**
5: Compute $\alpha_k \leftarrow \operatorname{argmin}_{\alpha \in \mathbb{R}} \; q(x_k + \alpha s_k)$
6: Set $x_{k+1} \leftarrow x_k + \alpha_k s_k$.
7: Set $r_{k+1} \leftarrow Ax_{k+1} - b$.
8: Pick new A-conjugate direction s_{k+1}.
9: Set $k \leftarrow k + 1$.
10: **end while**

- How do we compute α_k?
- How do we compute the A-conjugate directions efficiently?

Theorem 2.8 (general A-conjugate algorithm converges)

For any $x_0 \in \mathbb{R}^n$, the general A-conjugate direction Algorithm 5 computes the solution x^* of the system $Ax = b$ in at most n steps.

Proof: Theorem 5.1 in Nocedal and Wright.

Notes

Exercise: show that the α_k that solves the minimization problem on line 5 of Algorithm 5 satisfies

$$\alpha_k = -\frac{s_k^T r_k}{s_k^T A s_k}.$$

Before discussing how we compute the A-conjugate directions $\{s_i\}$, let us look at some properties of them if we assume we already have them.

Theorem 2.9 (Expanding subspace minimization)

Let $x_0 \in \mathbb{R}^n$ be any starting point and suppose that $\{x_k\}$ is the sequence of iterates generated by the A-conjugate direction Algorithm 5 for a set of A-conjugate directions $\{s_k\}$. Then,

$$r_k^T s_i = 0 \quad \text{for all } i = 0, \ldots k-1$$

and x_k is the unique minimizer of $q(x) = \frac{1}{2}x^T A x - b^T x$ over the set

$$\{x : x = x_0 + \text{span}(s_0, s_1, \ldots, s_{k-1})\}$$

Proof: See Theorem 5.2 in Nocedal and Wright.

Notes

Question: If $\{s_i\}_{i=0}^{k-1}$ are A-conjugate, how do we compute s_k to be A-conjugate?

Answer: Theorem 2.9 shows that r_k is orthogonal to the previously explored space. To keep it simple and hopefully cheap, let us try

$$s_k = -r_k + \beta s_{k-1} \quad \text{for some } \beta. \tag{5}$$

If this is going to work, then the A-conjugacy condition and (5) requires that

$$\begin{aligned} 0 &= s_{k-1}^T A s_k \\ &= s_{k-1}^T A(-r_k + \beta s_{k-1}) \\ &= s_{k-1}^T(-A r_k + \beta A s_{k-1}) \\ &= -s_{k-1}^T A r_k + \beta s_{k-1}^T A s_{k-1} \end{aligned}$$

and solving for β gives

$$\beta = \frac{s_{k-1}^T A r_k}{s_{k-1}^T A s_{k-1}}.$$

With this choice of β, the vector s_k is A-conjugate!.....but, how do we get started? Choosing $s_0 = -r_0$, i.e., a steepest descent direction, makes sense.

This gives us a complete algorithm; the linear CG algorithm!

Notes

Algorithm 6 Preliminary linear CG algorithm

input symmetric positive-definite matrix $A \in \mathbb{R}^{n \times n}$, and vectors x_0 and $b \in \mathbb{R}^n$.
Set $r_0 \leftarrow Ax_0 - b$, $s_0 \leftarrow -r_0$, and $k \leftarrow 0$.
while $r_k \neq 0$ **do**
  Set $\alpha_k \leftarrow -(s_k^T r_k)/(s_k^T A s_k)$.
  Set $x_{k+1} \leftarrow x_k + \alpha_k s_k$.
  Set $r_{k+1} \leftarrow Ax_{k+1} - b$.
  Set $\beta_{k+1} \leftarrow (s_k^T A r_{k+1})/(s_k^T A s_k)$.
  Set $s_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} s_k$.
  Set $k \leftarrow k + 1$.
end while

- This preliminary version requires two matrix-vector products per iteration.
- By using some more "tricks" and algebra, we can reduce this to a single matrix-vector multiplication per iteration.

Notes

Algorithm 7 Linear CG algorithm

input symmetric positive-definite matrix $A \in \mathbb{R}^{n \times n}$, and vectors x_0 and $b \in \mathbb{R}^n$.
Set $r_0 \leftarrow Ax_0 - b$, $s_0 \leftarrow -r_0$, and $k \leftarrow 0$.
while $r_k \neq 0$ **do**
  Set $\alpha_k \leftarrow (r_k^T r_k)/(s_k^T A s_k)$.
  Set $x_{k+1} \leftarrow x_k + \alpha_k s_k$.
  Set $r_{k+1} \leftarrow r_k + \alpha_k A s_k$.
  Set $\beta_{k+1} \leftarrow (r_{k+1}^T r_{k+1})/(r_k^T r_k)$.
  Set $s_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} s_k$.
  Set $k \leftarrow k + 1$.
end while

- Only requires the single matrix-vector multiplication As_k.
- More practical to use a stopping condition like

$$\|r_k\| \leq 10^{-8} \max\left(1, \|r_0\|_2\right)$$

- Required computation
  - **2** inner products
  - **3** vector sums
  - **1** matrix-vector multiplication
- Ideal for large (sparse) matrices A
- Converges quickly if $\mathbf{cond}(A)$ is small or the eigenvalues are "clustered"
  - convergence can be accelerated by using preconditioning

Notes

We want to use CG to compute an approximate solution p to

$$\underset{p\in\mathbb{R}^n}{\text{minimize}}\ f + g^T p + \tfrac{1}{2} p^T H p$$

- H may be indefinite (even singular) and must ensure that p is a descent direction

Algorithm 8 Newton CG algorithm for computing descent directions

1: **input** symmetric matrix $H \in \mathbb{R}^{n\times n}$ and vector g
2: Set $p_0 = 0$, $r_0 \leftarrow g$, $s_0 \leftarrow -g$, and $k \leftarrow 0$.
3: **while** $r_k \neq 0$ **do**
4: **if** $s_k^T H s_k > 0$ **then**
5: Set $\alpha_k \leftarrow (r_k^T r_k)/(s_k^T H s_k)$.
6: **else**
7: **if** $k = 0$, **then return** $p_k = -g$ **else return** p_k **end if**
8: **end if**
9: Set $p_{k+1} \leftarrow p_k + \alpha_k s_k$.
10: Set $r_{k+1} \leftarrow r_k + \alpha_k H s_k$.
11: Set $\beta_{k+1} \leftarrow (r_{k+1}^T r_{k+1})/(r_k^T r_k)$.
12: Set $s_{k+1} \leftarrow -r_{k+1} + \beta_{k+1} s_k$.
13: Set $k \leftarrow k + 1$.
14: **end while**
15: **return** p_k

Made the replacements $x \leftarrow p$, $A \leftarrow H$, and $b \leftarrow -g$ in Algorithm 7.

Notes

Theorem 2.10 (Newton CG algorithm computes descent directions.)

If $g \neq 0$ and Algorithm 8 terminates on iterate K, then every iterate p_k of the algorithm satisfies $p_k^T g < 0$ for $k \leq K$.

Proof:
Case 1: Algorithm 8 terminates on iteration $K = 0$.
It is immediate that $g^T p_0 = -g^T g = -\|g\|_2^2 < 0$ since $g \neq 0$.
Case 2: Algorithm 8 terminates on iteration $K \geq 1$.
First observe from $p_0 = 0$, $s_0 = -g$, $r_0 = g$, $g \neq 0$, and lines 10 and 9 of Algorithm 8 that

$$g^T p_1 = g^T(p_0 + \alpha_0 s_0) = \alpha_0 g^T s_0 = \frac{r_0^T r_0}{s_0^T H s_0} g^T s_0 = -\frac{\|g\|_2^4}{g^T H g} < 0. \tag{6}$$

By unrolling the "p" update, using A-conjugacy of $\{s_i\}$, and definition of r_k, we get

$$s_k^T r_k = s_k^T(H p_k + g) = s_k^T g + s_k^T H \sum_{j=0}^{k-1} \alpha_j s_j = s_k^T g.$$

The previous line, lines 9 and 5 of Algorithm 8, and the fact that $s_k^T r_k = -\|r_k\|_2^2$ gives

$$g^T p_{k+1} = g^T p_k + \alpha_k g^T s_k = g^T p_k + \alpha_k s_k^T r_k = g^T p_k + \frac{r_k^T r_k}{s_k^T H s_k} s_k^T r_k = g^T p_k - \frac{\|r_k\|_2^4}{s_k^T H s_k} < g^T p_k.$$

Combining the previous inequality and (6) results in

$$g^T p_{k+1} < g^T p_k < \cdots < g^T p_1 < -\frac{\|g\|_2^4}{g^T H g} < 0. \ \blacksquare$$

Notes

Algorithm 9 Backtracking

1: **input** x_k, p_k
2: Choose $\alpha_{\text{init}} > 0$ and $\tau \in (0,1)$
3: Set $\alpha^{(0)} = \alpha_{\text{init}}$ and $l = 0$
4: **until** $f(x_k + \alpha^{(l)} p_k)$ "$<$" $f(x_k)$
5: Set $\alpha^{(l+1)} = \tau \alpha^{(l)}$
6: Set $l \leftarrow l + 1$
7: **end until**
8: **return** $\alpha_k = \alpha^{(l)}$

- typical choices (not always)
  - $\alpha_{\text{init}} = 1$
  - $\tau = 1/2$
- this prevents the step from getting too small
- does not prevent the step from being too long
- decrease in f may not be proportional to the directional derivative
- need to tighten the requirement that

$$f(x_k + \alpha^{(l)} p_k) \text{ "}<\text{" } f(x_k)$$

Notes

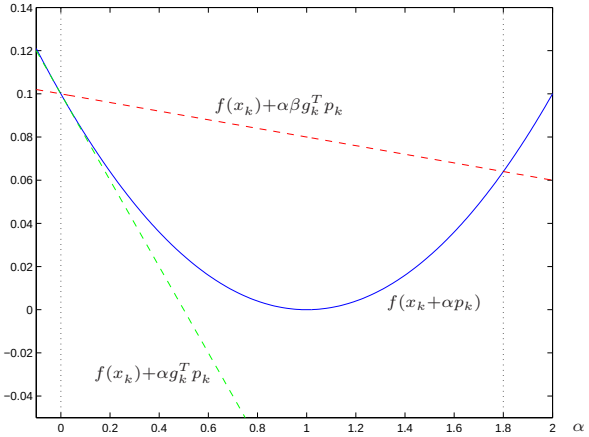
The Armijo condition

Given a point x_k and search direction p_k, we say that α_k satisfies the Armijo condition if

$$f(x_k + \alpha_k p_k) \leq f(x_k) + \eta \alpha_k g_k^T p_k \tag{7}$$

for some $\eta \in (0,1)$, e.g., $\eta = 0.1$ or even $\eta = 0.0001$

Purpose: ensure the decrease in f is substantial relative to the directional derivative.



Notes

Algorithm 10 A backtracking-Armijo linesearch

1: **input** x_k, p_k
2: Choose $\alpha_{\text{init}} > 0$, $\eta \in (0,1)$, and $\tau \in (0,1)$
3: Set $\alpha^{(0)} = \alpha_{\text{init}}$ and $l = 0$
4: **until** $f(x_k + \alpha^{(\ell)} p_k) \leq f(x_k) + \eta \alpha^{(\ell)} g_k^T p_k$
5: Set $\alpha^{(l+1)} = \tau \alpha^{(l)}$
6: Set $\ell \leftarrow \ell + 1$
7: **end until**
8: **return** $\alpha_k = \alpha^{(\ell)}$

- Does this always terminate?
- Does it give us what we want?

Notes

Theorem 3.1 (Satisfying the Armijo condition)

Suppose that

- $f \in C^1$ *and* $g(x)$ *is Lipschitz continuous with Lipschitz constant* $\gamma(x)$
- p *is a descent direction at* x

Then for any given $\eta \in (0,1)$*, the Armijo condition*

$$f(x + \alpha p) \leq f(x) + \eta \alpha\, g(x)^T p$$

is satisfied for all $\alpha \in [0, \alpha_{\max}(x)]$*, where*

$$\alpha_{\max}(x) := \frac{2(\eta - 1) g(x)^T p}{\gamma(x) \|p\|_2^2} > 0$$

Proof:
A Taylor's approximation and

$$\alpha \leq \frac{2(\eta - 1) g(x)^T p}{\gamma(x) \|p\|_2^2}$$

imply that

$$\begin{aligned} f(x + \alpha p) &\leq f(x) + \alpha g(x)^T p + \tfrac{1}{2} \gamma(x) \alpha^2 \|p\|_2^2 \\ &\leq f(x) + \alpha g(x)^T p + \alpha(\eta - 1) g(x)^T p \\ &= f(x) + \alpha \eta\, g(x)^T p \qquad \blacksquare \end{aligned}$$

Notes

Theorem 3.2

[Bound on α_k when using an Armijo backtracking linesearch] Suppose that

- $f \in C^1$ *and* $g(x)$ *is Lipschitz continuous with Lipschitz constant* γ_k *at* x_k
- p_k *is a descent direction at* x_k

Then for any chosen $\eta \in (0, 1)$ *the stepsize* α_k *generated by the backtracking-Armijo linesearch terminates with*

$$\alpha_k \geq \min\left(\alpha_{init}, \frac{2\tau(\eta - 1)g_k^T p_k}{\gamma_k \|p_k\|_2^2}\right) \equiv \min\left(\alpha_{init}, \tau\alpha_{max}(x_k)\right)$$

where $\tau \in (0, 1)$ *is the backtracking parameter.*

Proof:

Theorem 3.1 implies that the backtracking will terminate as soon as $\alpha^{(l)} \leq \alpha_{\max}(x_k)$. Consider the following two cases:

- α_{init} satisfies the Armijo condition: it is then clear that $\alpha_k = \alpha_{\text{init}}$.
- α_{init} does not satisfy the Armijo condition: thus, there must be a last linesearch iterate (the l-th) for which

$$\alpha^{(l)} > \alpha_{\max}(x_k) \quad \Longrightarrow \quad \alpha_k = \alpha^{(l+1)} = \tau\alpha^{(l)} > \tau\alpha_{\max}(x_k)$$

Combining the two cases gives the required result. ∎

Notes

Algorithm 11 Generic backtracking-Armijo linesearch method

1: **input** initial guess x_0
2: Set $k = 0$
3: **loop**
4: Find a descent direction p_k at x_k.
5: Compute the stepsize α_k using the backtracking-Armijo linesearch Algorithm 10.
6: Set $x_{k+1} = x_k + \alpha_k p_k$
7: Set $k \leftarrow k + 1$
8: **end loop**
9: **return** approximate solution x_k

- should include a sensible relative stopping tolerance such as

$$\|\nabla f(x_k)\| \leq 10^{-8} \max\left(1, \|\nabla f(x_0)\|\right)$$

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Theorem 3.3 (Global convergence of generic backtracking-Armijo linesearch)

Suppose that

- $f \in C^1$
- g *is Lipschitz continuous on* $\mathbb{R}^n$ *with Lipschitz constant* γ

Then, the iterates generated by the generic backtracking-Armijo linesearch method Algorithm 11 must satisfy one of the following conditions:

1. *finite termination, i.e., there exists a positive integer* k *such that*

$$g_k = 0 \quad \text{for some} \quad k \geq 0$$

2. *objective is unbounded below, i.e.,*

$$\lim_{k \to \infty} f_k = -\infty$$

3. *an angle condition between* g_k *and* p_k *exists, i.e.,*

$$\lim_{k \to \infty} \min \left(|p_k^T g_k|, |p_k^T g_k|^2 / \|p_k\|_2^2 \right) = 0$$

Notes

Proof:

Suppose that outcomes **1** and **2** do not happen, i.e., $g_k \neq 0$ for all $k \geq 0$ and

$$\lim_{k \to \infty} f_k > -\infty. \tag{8}$$

The Armijo condition implies that

$$f_{k+1} - f_k \leq \eta \alpha_k p_k^T g_k$$

for all k. Summing over the first j iterations yields

$$f_{j+1} - f_0 \leq \eta \sum_{k=0}^{j} \alpha_k p_k^T g_k \tag{9}$$

Taking limits of the previous inequality as $j \to \infty$ and using (8) implies that the LHS is bounded below and, therefore, the RHS is also bounded below. Since the sum is composed of all negative terms, we deduce that the following sum

$$\sum_{k=0}^{\infty} \alpha_k |p_k^T g_k| \tag{10}$$

is bounded.

Notes

From Theorem 3.2, $\alpha_k \geq \min\left\{\alpha_{init}, \frac{2\tau(\eta-1)g_k^T p_k}{\gamma\|p_k\|_2^2}\right\}$. Thus,

$$\begin{aligned}\sum_{k=0}^{\infty} \alpha_k |p_k^T g_k| &\geq \sum_{k=0}^{\infty} \min\left\{\alpha_{init}, \frac{2\tau(\eta-1)g_k^T p_k}{\gamma\|p_k\|_2^2}\right\} |p_k^T g_k| \\ &= \sum_{k=0}^{\infty} \min\left\{\alpha_{init}|p_k^T g_k|, \frac{2\tau(1-\eta)|p_k^T g_k|^2}{\gamma\|p_k\|_2^2}\right\} \\ &\geq \sum_{k=0}^{\infty} \min\{\alpha_{init}, \tfrac{2\tau(1-\eta)}{\gamma}\} \min\left\{|p_k^T g_k|, \tfrac{|p_k^T g_k|^2}{\|p_k\|_2^2}\right\}\end{aligned}$$

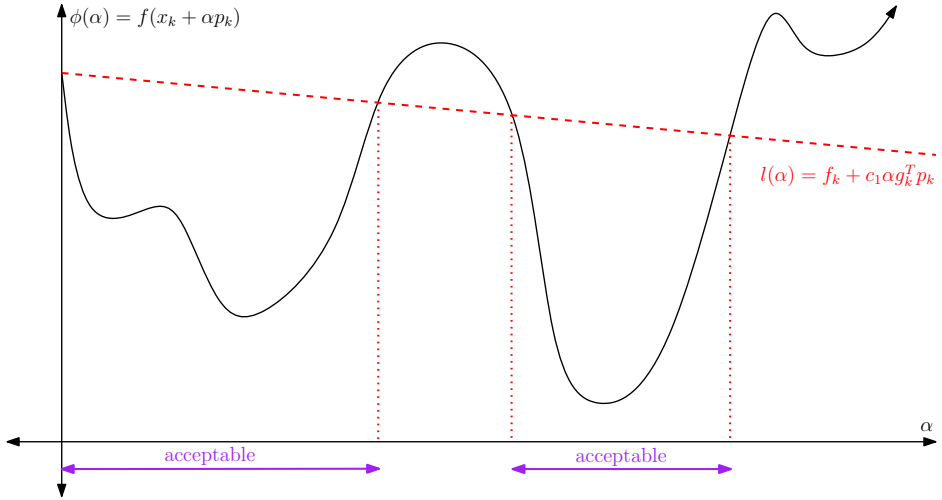
Using the fact that the series (10) converges, we obtain that

$$\lim_{k\to\infty} \min\left(|p_k^T g_k|, |p_k^T g_k|^2/\|p_k\|_2^2\right) = 0$$

Notes

Some observations

- the Armijo condition prevents too “long” of steps
- typically, the Armijo condition is satisfied for very “large” intervals
- the Armijo condition can be satisfied by steps that are not even close to a minimizer of $\phi(x) := f(x_k + \alpha p_k)$



Notes

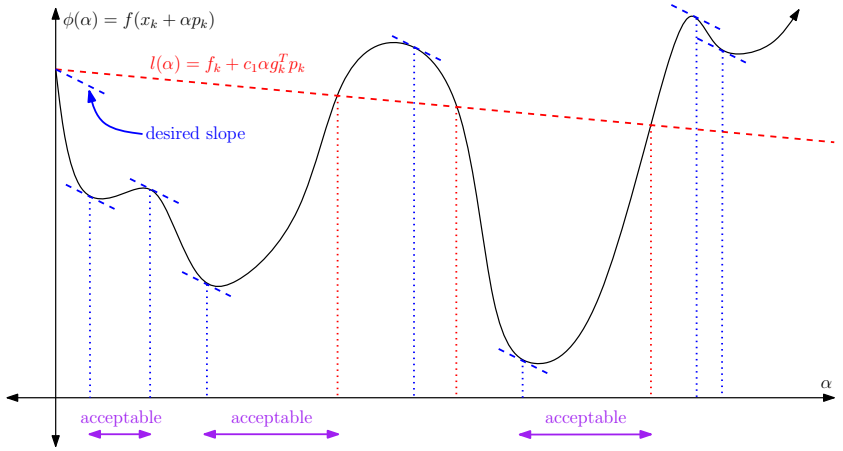
Wolfe conditions

Given the current iterate x_k, search direction p_k, and constants $0 < c_1 < c_2 < 1$, we say that the step length α_k satisfies the Wolfe conditions if

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f(x_k)^T p_k \tag{11a}$$

$$\nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f(x_k)^T p_k \tag{11b}$$

- condition (11a) is the Armijo condition (ensures "sufficient" decrease)
- condition (11b) is a directional derivative condition (prevents too short of steps)



Notes

Algorithm 12 Generic Wolfe linesearch method

1: **input** initial guess x_0
2: Set $k = 0$
3: **loop**
4: Find a descent direction p_k at x_k.
5: Compute a stepsize α_k that satisfies the Wolfe conditions (11).
6: Set $x_{k+1} = x_k + \alpha_k p_k$
7: Set $k \leftarrow k + 1$
8: **end loop**
9: **return** approximate solution x_k

- should include a sensible relative stopping tolerance such as

$$\|\nabla f(x_k)\| \leq 10^{-8} \max\left(1, \|\nabla f(x_0)\|\right)$$

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Theorem 3.4 (Convergence of generic Wolfe linesearch (Zoutendijk))

Assume that

- $f : \mathbb{R}^n \to \mathbb{R}$ *is bounded below on* $\mathcal{C}^1$ *on* $\mathbb{R}^n$
- $\nabla f(x)$ *is Lipschitz continous on* $\mathbb{R}^n$ *with constant* L

It follows that the iterates generated from the generic Wolfe linesearch method satisfy

$$\sum_{k \geq 0} \cos^2(\theta_k) \|g_k\|_2^2 < \infty \tag{12}$$

where

$$\cos(\theta_k) \stackrel{\text{def}}{=} \frac{-g_k^T p_k}{\|g_k\|_2 \|p_k\|_2} \tag{13}$$

Comments

- definition (13) measures the angle between the gradient g_k and search direction p_k
  - $\cos(\theta) \approx 0$ implies g_k and p_k are nearly orthogonal
  - $\cos(\theta) \approx 1$ implies g_k and p_k are nearly parallel
- condition (12) ensures that the gradient converges to zero provided g_k and p_k stay away from being arbitrarily close to orthogonal

Proof: See Theorem 3.2 in Nocedal and Wright.

Notes

Some comments

- The Armijo linesearch
  - only requires function evaluations
  - may easily accept steps that are far from a univariate minimizer of $\phi(\alpha) = f(x_k + \alpha p_k)$
- The Wolfe linesearch
  - requires function and gradient evaluations
  - typically produces steps that are closer to the univariate minimizer of ϕ
  - may still allow the acceptance of steps that are far from a univariate minimizer of ϕ
  - "ideal" when seach directions are computed from linear systems based on the BFGS quasi-Newton updating formula

Note: we have not yet said how to compute steps that satisfy the Wolfe conditions. We have not even shown that such steps exist! (coming soon)

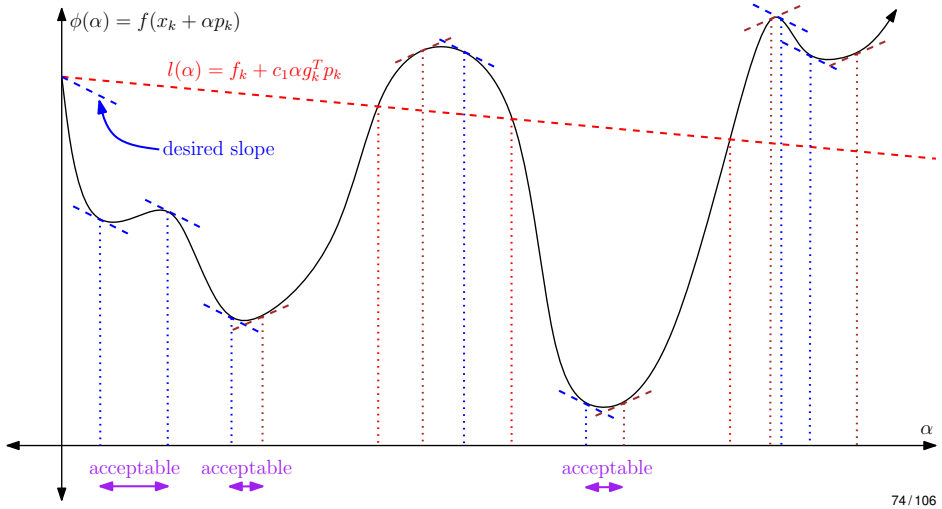
Notes

Strong Wolfe conditions

Given the current iterate x_k, search direction p_k, and constants $0 < c_1 < c_2 < 1$, we say that the step length α_k satisfies the Strong Wolfe conditions if

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f(x_k)^T p_k \tag{14a}$$

$$|\nabla f(x_k + \alpha_k p_k)^T p_k| \leq c_2 |\nabla f(x_k)^T p_k| \tag{14b}$$



Notes

Theorem 3.5

Suppose that $f \in \mathbb{R}^n \to \mathbb{R}$ is in C^1 and p_k is a descent direction at x_k, and assume that f is bounded below along the ray $\{x_k + \alpha p_k : \alpha > 0\}$. It follows that if $0 < c_1 < c_2 < 1$, then there exist nontrivial intervals of step lengths that satisfy the strong Wolfe conditions (14).

Proof:

The function $\phi(\alpha) := f(x_k + \alpha p_k)$ is bounded below over $\alpha > 0$ by assumption and must, therefore, intersect the graph of $l(\alpha) := f(x_k) + \alpha c_1 \nabla f(x_k)^T p_k$ at least once since $c_1 \in (0, 1)$; let $\alpha_{\min} > 0$ be the smallest such intersecting value so that

$$f(x_k + \alpha_{\min} p_k) = f(x_k) + \alpha_{\min} c_1 \nabla f(x_k)^T p_k. \tag{15}$$

It is clear that (11a)/(14a) hold for all $\alpha \in (0, \alpha_{\min}]$. The Mean Value Theorem now implies

$$f(x_k + \alpha_{\min} p_k) - f(x_k) = \alpha_{\min} \nabla f(x_k + \alpha_M p_k)^T p_k \quad \text{for some } \alpha_M \in (0, \alpha_{\min}).$$

Combining the last equality with (15) and the facts that $c_1 < c_2$ and $\nabla f(x_k)^T p_k < 0$ yield

$$\nabla f(x_k + \alpha_M p_k)^T p_k = c_1 \nabla f(x_k)^T p_k > c_2 \nabla f(x_k)^T p_k. \tag{16}$$

Thus, α_M satisfies (11a)/(14a) and (11b) with a strict inequality so we may use the smoothness assumption to deduce that there is an interval around α_M for which (11) and (14a) hold. Finally, since the left-hand-side of (16) is negative, we also know that (14b) holds, which completes the proof. ∎

Notes

Algorithm 13 A bisection type (weak) Wolfe linesearch

input $x_k, p_k, 0 < c_1 < c_2 < 1$
Choose $\alpha = 0, t = 1$, and $\beta = \infty$
while $(f(x_k + tp_k) > f(x_k) + c_1 \cdot t \cdot (g_k^T p_k)$ **OR** $\nabla f(x_k + tp_k)^T p_k < c_2(g_k^T p_k))$ **do**
  if $f(x_k + tp_k) > f(x_k) + c_1 \cdot t \cdot (g_k^T p_k)$ **then**
    Set $\beta := t$
    Set $t := \frac{\alpha+\beta}{2}$
  else
    $\alpha := t$
    if $\beta = \infty$ **then**
      $t := 2\alpha$
    else
      $t := \frac{\alpha+\beta}{2}$
    end if
  end if
end while

return t

See Section 3.5 in Nocedal-Wright for more discussions; in particular, a procedure for the strong Wolfe conditions.

Notes

Some comments

- The Armijo linesearch
  - only requires function evaluations
  - computationally cheapest to implement
  - may easily accept steps that are far from a univariate minimizer of $\phi(\alpha) = f(x_k + \alpha p_k)$
- The Wolfe linesearch
  - requires function and gradient evaluations
  - typically produces steps that are closer to the univariate minimizer of ϕ
  - may still allow the acceptance of steps that are far from a univariate minimizer of ϕ
  - computationally more expensive to implement compared to Armijo
- The strong Wolfe linesearch
  - requires function and gradient evaluations
  - typically produces steps that are closer to the univariate minimizer of ϕ
  - only approximate stationary points of the univariate function ϕ satisfy these conditions.
  - computationally most expensive to implement compared to Armijo

Why use (strong) Wolfe conditions?

- sometimes more accurate line search lead to fewer outer (major) iterations of the linesearch method.
- beneficial in the context of quasi-Newton methods for maintaining positive-definite matrix approximations.

Notes

Theorem 3.6 (Wolfe conditions guarantee the BFGS update is well-defined)

Suppose that $B_k \succ 0$ and that p_k is a descent direction for f at x_k. If a (strong) Wolfe linesearch is used to compute α_k such that $x_{k+1} = x_k + \alpha_k p_k$, then

$$y_k^T s_k > 0$$

where

$$s_k = x_{k+1} - x_k = \alpha_k p_k \quad \text{and} \quad y_k = g_{k+1} - g_k.$$

Proof:

It follows from (11b) that

$$\nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f(x_k)^T p_k.$$

Multplying both sides by α_k, using $x_{k+1} = x_k + \alpha_k p_k$, and notation $g_k = \nabla f(x_k)$, yields

$$g_{k+1}^T s_k \geq c_2 g_k^T s_k.$$

Subtracting $g_k^T s_k$ from both sides gives

$$g_{k+1}^T s_k - g_k^T s_k \geq c_2 g_k^T s_k - g_k^T s_k$$

so that

$$y_k^T s_k \geq (c_2 - 1) g_k^T s_k = \alpha_k (c_2 - 1) g_k^T p_k > 0$$

since $c_2 \in (0, 1)$ and p_k is a descent direction for f at x_k. ∎

Notes

Algorithm 14 Steepest descent backtracking-Armijo linesearch method

1: Input: initial guess x_0
2: Set $k = 0$
3: **until** $\|\nabla f(x_k)\| \leq 10^{-8} \max(1, \|\nabla f(x_0)\|)$
4: Set $p_k = -\nabla f(x_k)$ as the search direction.
5: Compute the stepsize α_k using the backtracking-Armijo linesearch Algorithm 10.
6: Set $x_{k+1} = x_k + \alpha_k p_k$
7: Set $k \leftarrow k + 1$
8: **end until**
9: **return** approximate solution x_k

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Theorem 4.1 (Global convergence for steepest descent)

If $f \in \mathcal{C}^1$ and g is Lipschitz continuous on $\mathbb{R}^n$, then the iterates generated by the steepest-descent backtracking-Armijo linesearch Algorithm 14 satisfies one of the following conditions:

1. *finite termination, i.e., there exists some finite integer $k \geq 0$ such that*
$$g_k = 0$$
2. *objective is unbounded below, i.e.,*
$$\lim_{k \to \infty} f_k = -\infty$$
3. *convergence of gradients, i.e.,*
$$\lim_{k \to \infty} g_k = 0$$

Proof:

Since $p_k = -g_k$, if outcome 1 above does not happen, then we may conclude that

$$\|g_k\| = \|p_k\| \neq 0 \quad \text{for all } k \geq 0$$

Additionally, if outcome 2 above does not occur, then Theorem 3.3 ensures that

$$0 = \lim_{k \to \infty} \left\{ \min \left(|p_k^T g_k|, |p_k^T g_k|^2 / \|p_k\|_2^2 \right) \right\} = \lim_{k \to \infty} \{ \|g_k\|_2 \min (\|g_k\|_2, 1) \}$$

and thus $\lim_{k \to \infty} g_k = 0$. ∎

Notes

Some general comments on the steepest descent backtracking-Armijo algorithm

- archetypal globally convergent method
- many other methods resort to steepest descent when things “go wrong”
- not scale invariant
- convergence is usually slow! (linear local convergence, possibly with constant close to 1; for global convergence only sublinear rate $O((\frac{1}{\epsilon})^2)$ to get to a “stationary" point, i.e., $\|g_k\| \leq \epsilon$)
- in practice, often does not converge at all
- slow convergence results because the computation of p_k does not use any curvature information
- call any method that uses the steepest descent direction a “method of steepest descent”
- each iteration is relatively cheap, but you may need many of them!

Notes

Rate of convergence

Theorem 4.2 (Global convergence rate for steepest-descent)

Suppose $f \in \mathcal{C}^1$ and ∇f is Lipschitz continuous on $\mathbb{R}^n$. Further assume that $f(x)$ is bounded from below on $\mathbb{R}^n$. Let $\{x_k\}$ be the iterates generated by the steepest-descent backtracking-Armijo linesearch Algorithm 14. Then there exists a constant M such that for all $T \geq 1$

$$\min_{k=0,\ldots,T} \|\nabla f(x_k)\| \leq \frac{M}{\sqrt{T+1}}.$$

Consequently, for any $\epsilon > 0$, within $\lceil \left(\frac{M}{\epsilon}\right)^2 \rceil$ steps, we will see an iterate where the gradient has norm at most ϵ. In other words, we reach an "ϵ-stationary" point in $O((\frac{1}{\epsilon})^2)$ steps

REMARK: Same thing holds for constant step size for an appropriately chosen constant. See HW.

Proof:

Recall (9) in the proof of Theorem 3.3:

$$\sum_{k=0}^{T} \alpha_k |g_k^T p_k| \leq \frac{f_0 - f_{k+1}}{\eta} \leq M' \qquad \text{since } f \text{ is bounded from below.}$$

Notes

Rate of convergence

Thus,

$$\sum_{k:\tau\alpha_{\max} < \alpha_{init}} \frac{2\tau(1-\eta)|g_k^T p_k|^2}{\gamma \|p_k\|^2} + \sum_{k:\tau\alpha_{\max} \geq \alpha_{init}} \alpha_{init} |g_k^T p_k| \leq M'.$$

Thus,

$$\sum_{k:\tau\alpha_{\max} < \alpha_{init}} \frac{|g_k^T p_k|^2}{\|p_k\|^2} + \sum_{k:\tau\alpha_{\max} \geq \alpha_{init}} |g_k^T p_k| \leq \frac{M'}{C}, \tag{17}$$

where $C = \min\left\{\frac{2\tau(1-\eta)}{\gamma}, \alpha_{init}\right\}$.

Setting $p_k = -g_k$ in the inequality above, we obtain that

$$(T+1) \min_{k=0,\ldots,T} \|g_k\|^2 \leq \sum_{k=0,\ldots,T} \|g_k\|^2 \leq \frac{M'}{C}.$$

Therefore,

$$\min_{k=0,\ldots,T} \|g_k\| \leq \frac{M}{\sqrt{T+1}},$$

for some constant M. ∎

Notes

Steepest descent example

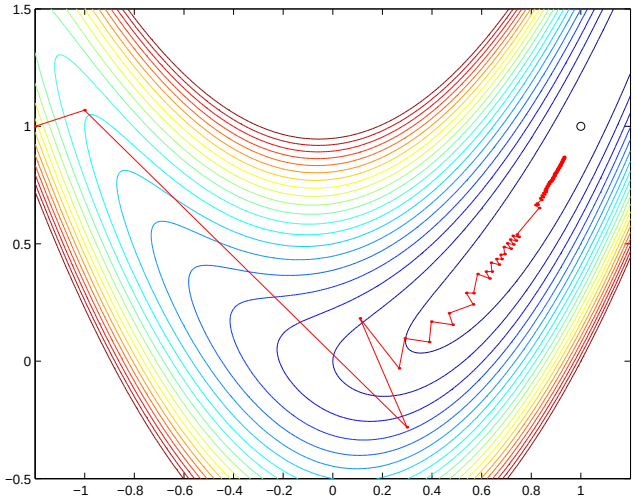


Figure: Contours for the objective function $f(x,y) = 10(y-x^2)^2 + (x-1)^2$, and the iterates generated by the steepest-descent backtracking-Armijo linesearch Algorithm 14.

Notes

Rate of convergence

Theorem 4.3 (Local convergence rate for steepest-descent)

Suppose the following all hold:

- *f is twice continuously differentiable and $\nabla^2 f$ is Lipschitz continuous on $\mathbb{R}^n$ with Lipschitz constant M.*
- *x^* is a local minimum of f with positive definite Hessian $\nabla^2 f(x^*)$ with eigenvalues lower bounded by ℓ and upper bounded by L.*
- *The initial starting iterate x_0 is close enough to x^*; more precisely, $r_0 := \|x_0 - x^*\| < \bar{r} := \frac{2\ell}{M}$.*

The steepest-descent with constant step size $\alpha = \frac{2}{\ell+L}$ converges as follows:

$$\|x_k - x^*\| \leq \frac{\bar{r} r_0}{\bar{r} - r_0}\left(1 - \frac{2\ell}{L+3\ell}\right)^k.$$

In other words, in $O(\log(\frac{1}{\epsilon}))$ iterations, we are within a distance of ϵ from x^*.

Proof: See Theorem 1.2.4 in Nesterov's book.

See also Theorem 3.4 in Nocedal-Wright for a similar result with exact line-search.

Notes

Algorithm 15 Modified-Newton backtracking-Armijo linesearch method

Input: initial guess x_0
Set $k = 0$
until $\|\nabla f(x_k)\| \leq 10^{-8} \max(1, \|\nabla f(x_0)\|)$
  Compute positive-definite matrix B_k from H_k using Algorithm 2.
  Compute the search direction p_k as the solution to $B_k p = -g_k$.
  Compute the stepsize α_k using the backtracking-Armijo linesearch Algorithm 10.
  Set $x_{k+1} = x_k + \alpha_k p_k$
  Set $k \leftarrow k + 1$
end until
return approximate solution x_k

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Theorem 4.4 (Global convergence of modifed-Newton backtracking-Armijo)

Suppose that

- $f \in C^1$
- g *is Lipschitz continuous on* $\mathbb{R}^n$
- *the eigenvalues of* B_k *are uniformly bounded away from zero and infinity*

Then, the iterates generated by the modified-Newton backtracking-Armijo Algorithm 15 satisfy one of the following:

1. *finite termination, i.e., there exists a finite* k *such that*
$$g_k = 0$$
2. *objective is unbounded below, i.e.,*
$$\lim_{k \to \infty} f_k = -\infty$$
3. *convergence of gradients, i.e.,* $\lim_{k \to \infty} g_k = 0$

Proof:
Let $\lambda_{\min}(B_k)$ and $\lambda_{\max}(B_k)$ be the smallest and largest eigenvalues of B_k. By assumption, there are bounds $0 < \lambda_{\min} \leq \lambda_{\max}$ such that

$$\lambda_{\min} \leq \lambda_{\min}(B_k) \leq \frac{s^T B_k s}{\|s\|^2} \leq \lambda_{\max}(B_k) \leq \lambda_{\max} \quad \text{for any nonzero } s.$$

Notes

From the previous slide, it follows that

$$\lambda_{\max}^{-1} \leq \lambda_{\max}^{-1}(B_k) = \lambda_{\min}(B_k^{-1}) \leq \frac{s^T B_k^{-1} s}{\|s\|^2} \leq \lambda_{\max}(B_k^{-1}) = \lambda_{\min}^{-1}(B_k) \leq \lambda_{\min}^{-1} \tag{18}$$

for any nonzero vector s. Using $B_k p_k = -g_k$ and (18) we see that

$$|p_k^T g_k| = |g_k^T B_k^{-1} g_k| \geq \lambda_{\max}^{-1} \|g_k\|_2^2 \tag{19}$$

In addition, we may use (18) to see that

$$\|p_k\|_2^2 = g_k^T B_k^{-2} g_k \leq \lambda_{\min}^{-2} \|g_k\|_2^2,$$

which implies that

$$\|p_k\|_2 \leq \lambda_{\min}^{-1} \|g_k\|_2.$$

It now follows from the previous inequality and (19) that

$$\frac{|p_k^T g_k|}{\|p_k\|_2} \geq \frac{\lambda_{\min}}{\lambda_{\max}} \|g_k\|_2. \tag{20}$$

Combining the previous inequality and (19) yields

$$\min\left(|p_k^T g_k|, |p_k^T g_k|^2 / \|p_k\|_2^2\right) \geq \frac{\|g_k\|_2^2}{\lambda_{\max}} \min\left(1, \frac{\lambda_{\min}^2}{\lambda_{\max}}\right). \tag{21}$$

From Theorem 3.3 we know that $\lim_{k\to\infty} \min\left(|p_k^T g_k|, |p_k^T g_k|^2 / \|p_k\|_2^2\right) = 0$ and combined with (21), we conclude that

$$\lim_{k\to\infty} g_k = 0. \qquad \blacksquare$$

Notes

Rate of convergence

Theorem 4.5 (Global convergence rate for modified-Newton)

Suppose $f \in C^1$ and ∇f is Lipschitz continuous on $\mathbb{R}^n$. Further assume that $f(x)$ is bounded from below on $\mathbb{R}^n$. Let $\{x_k\}$ be the iterates generated by the modified-Newton backtracking-Armijo linesearch Algorithm 15 such that B_k has eigenvalues uniformly bounded away from 0 and infinity. Then there exists a constant M such that for all $T \geq 1$

$$\min_{k=0,\ldots,T} \|\nabla f(x_k)\| \leq \frac{M}{\sqrt{T+1}}.$$

Consequently, for any $\epsilon > 0$, within $\lceil \left(\frac{M}{\epsilon}\right)^2 \rceil$ steps, we will see an iterate where the gradient has norm at most ϵ. In other words, we reach an "ϵ-stationary" point in $O((\frac{1}{\epsilon})^2)$ steps

Proof: Almost identical to steepest descent proof (Theorem 4.2); use (19) and (20) in (17).

REMARK: Same thing holds for constant step size for an appropriately chosen constant.

Notes

Rate of convergence

Theorem 4.6 (Local quadratic convergence for modified-Newton)

Suppose that

- $f \in \mathcal{C}^2$
- H *is Lipschitz continuous on* $\mathbb{R}^n$ *with constant* γ

Suppose that iterates are generated from the modified-Newton backtracking-Armijo Algorithm 15 such that

- $\alpha_{init} = 1$
- $\eta \in (0, \frac{1}{2})$
- $B_k = H_k$ *whenever* H_k *is positive definite*

If the sequence of iterates $\{x_k\}$ *has a limit point* x^* *satisfying* $H(x^*)$ *is positive definite, then it follows that*

(i) $\alpha_k = 1$ *for all sufficiently large* k,

(ii) *the entire sequence* $\{x_k\}$ *converges to* x^*, *and*

(iii) *the rate of convergence is q-quadratic, i.e, there is a constant* $\kappa \geq 0$ *and a natural number* k_0 *such that for all* $k \geq k_0$

$$\|x_{k+1} - x^*\|_2 \leq \kappa \|x_k - x^*\|_2^2$$

Notes

Proof:
By assumption we know that there is some subsequence $\mathcal{K}$ such that

$$\lim_{k \in \mathcal{K}} x_k = x^* \quad \text{and} \quad H(x^*) \succ 0$$

Continuity implies that H_k is positive definite for all $k \in \mathcal{K}$ sufficiently large so that

$$p_k^T H_k p_k \geq \tfrac{1}{2} \lambda_{\min}(H(x^*)) \|p_k\|_2^2 \quad \text{for all } k_0 \leq k \in \mathcal{K} \tag{22}$$

for some k_0, where $\lambda_{\min}(H(x^*))$ is the smallest eigenvalue of $H(x^*)$. This fact and since $H_k p_k = -g_k$ for $k_0 \leq k \in \mathcal{K}$ implies that

$$|p_k^T g_k| = -p_k^T g_k = p_k^T H_k p_k \geq \tfrac{1}{2} \lambda_{\min}(H(x^*)) \|p_k\|_2^2 \quad \text{for all } k_0 \leq k \in \mathcal{K}. \tag{23}$$

This also implies

$$\frac{|p_k^T g_k|}{\|p_k\|_2} \geq \tfrac{1}{2} \lambda_{\min}(H(x^*)) \|p_k\|_2. \tag{24}$$

We now deduce from Theorem 3.3, (23), and (24) that

$$\lim_{k \in \mathcal{K} \to \infty} p_k = 0.$$

Notes

Mean Value Theorem implies that there exists z_k between x_k and $x_k + p_k$ such that

$$f(x_k + p_k) = f_k + p_k^T g_k + \tfrac{1}{2} p_k^T H(z_k) p_k.$$

Lipschitz continuity of $H(x)$ and the fact that $H_k p_k = -g_k$ implies

$$\begin{aligned} f(x_k + p_k) - f_k - \tfrac{1}{2} p_k^T g_k &= \tfrac{1}{2}(p_k^T g_k + p_k^T H(z_k) p_k) \\ &= \tfrac{1}{2} p_k^T (H(z_k) - H_k) p_k \\ &\leq \tfrac{1}{2} \|H(z_k) - H(x_k)\|_2 \|p_k\|_2^2 \leq \tfrac{1}{2}\gamma \|p_k\|_2^3. \end{aligned} \tag{25}$$

Since $\eta \in (0, 1/2)$ and $p_k \to 0$, we may pick k sufficiently large so that

$$2\gamma \|p_k\|_2 \leq \lambda_{\min}(H(x^*))(1 - 2\eta). \tag{26}$$

Combining (25), (26), and (23) shows that

$$\begin{aligned} f(x_k + p_k) - f_k &\leq \tfrac{1}{2} p_k^T g_k + \tfrac{1}{2}\gamma \|p_k\|_2^3 \\ &\leq \tfrac{1}{2} p_k^T g_k + \tfrac{1}{4} \lambda_{\min}(H(x^*))(1 - 2\eta) \|p_k\|_2^2 \\ &\leq \tfrac{1}{2} p_k^T g_k - \tfrac{1}{2}(1 - 2\eta) p_k^T g_k \\ &= \eta p_k^T g_k \end{aligned}$$

so that the unit step $x_k + p_k$ satisfies the Armijo condition for all $k \in \mathcal{K}$ sufficiently large.

Notes

Note that (22) implies that

$$\|H_k^{-1}\|_2 \leq 2/\lambda_{\min}(H(x^*)) \quad \text{for all } k_0 \leq k \in \mathcal{K}. \tag{27}$$

The iteration gives

$$\begin{aligned} x_{k+1} - x^* &= x_k - x^* - H_k^{-1} g_k = x_k - x^* - H_k^{-1}(g_k - g(x^*)) \\ &= H_k^{-1}\left[g(x^*) - g_k - H_k(x^* - x_k)\right]. \end{aligned}$$

But a Taylor Approximation provides the estimate

$$\|g(x^*) - g_k - H_k(x^* - x_k)\|_2 \leq \frac{\gamma}{2} \|x_k - x^*\|_2^2$$

which implies

$$\|x_{k+1} - x^*\|_2 \leq \frac{\gamma}{2} \|H_k^{-1}\|_2 \|x_k - x^*\|_2^2 \leq \frac{\gamma}{\lambda_{\min}(H(x^*))} \|x_k - x^*\|_2^2 \tag{28}$$

Thus, we know that for $k \in \mathcal{K}$ sufficiently large, the unit step will be accepted and

$$\|x_{k+1} - x^*\|_2 \leq \tfrac{1}{2} \|x_k - x^*\|_2$$

which proves parts (i) and (ii) since the entire argument may be repeated. Finally, part (iii) then follows from part (ii) and (28) with the choice

$$\kappa = \gamma / \lambda_{\min}(H(x^*))$$

which completes the proof. ∎

Notes

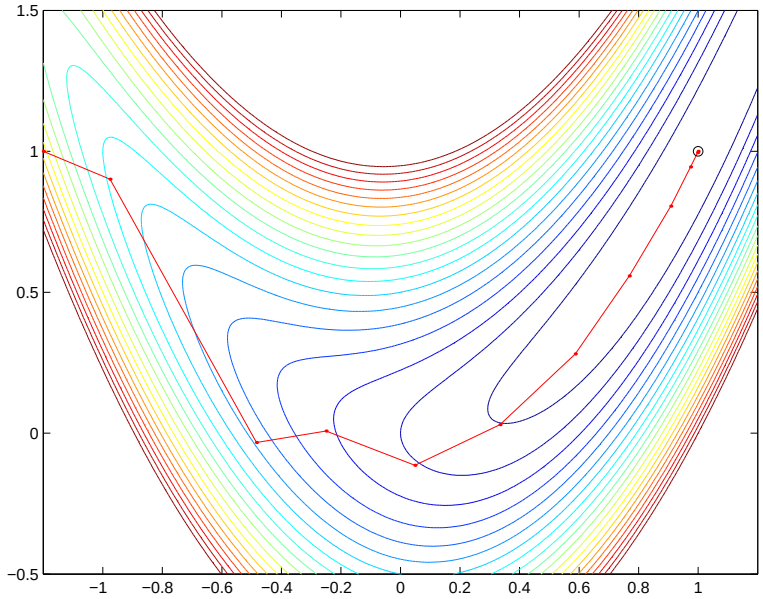


Figure: Contours for the objective function $f(x,y) = 10(y - x^2)^2 + (x-1)^2$, and the iterates generated by the modified-Newton backtracking-Armijo Algorithm 15.

Notes

Algorithm 16 Modified-Newton Wolfe linesearch method

Input: initial guess x_0
Set $k = 0$
until $\|\nabla f(x_k)\| \leq 10^{-8} \max\left(1, \|\nabla f(x_0)\|\right)$
  Compute positive-definite matrix B_k from H_k using Algorithm 2.
  Compute a search direction p_k as the solution to $B_k p = -g_k$.
  Compute a stepsize α_k that satisfies the Wolfe conditions (11a) and (11b).
  Set $x_{k+1} \leftarrow x_k + \alpha_k p_k$
  Set $k \leftarrow k + 1$
end until
return approximate solution x_k

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Algorithm 17 Quasi-Newton Wolfe linesearch method

Input: initial guess x_0
Set $k = 0$
until $\|\nabla f(x_k)\| \leq 10^{-8} \max(1, \|\nabla f(x_0)\|)$
  Compute positive-definite matrix B_k from B_{k-1} using the BFGS rule, or using Algorithm 3 with a seed matrix B_k^0.
  Compute a search direction p_k as the solution to $B_k p = -g_k$.
  Compute a stepsize α_k that satisfies the Wolfe conditions (11a) and (11b).
  Set $x_{k+1} \leftarrow x_k + \alpha_k p_k$
  Set $k \leftarrow k + 1$
end until
return approximate solution x_k

- should also terminate if a maximum number of allowed iterations is reached
- should also terminate if a maximum time limit is reached

Notes

Theorem 4.7 (Global convergence of modifed-Newton/quasi-Newton Wolfe)

Suppose that

- $f \in C^1$
- g *is Lipschitz continuous on* $\mathbb{R}^n$
- *the condition number of* B_k *is uniformly bounded by* β

Then, the iterates generated by the modified/quasi-Newton Wolfe Algorithm 17 or 16 satisfy one of the following:

1. *finite termination, i.e., there exists a finite* k *such that*
$$g_k = 0$$
2. *objective is unbounded below, i.e.,*
$$\lim_{k \to \infty} f_k = -\infty$$
3. *convergence of gradients, i.e.,*
$$\lim_{k \to \infty} g_k = 0$$

Proof:
Homework assignment.

Notes

Rate of convergence

Theorem 4.8 (Global convergence rate for modified-Newton/quasi-Newton Wolfe)

Suppose $f \in \mathcal{C}^1$ and ∇f is Lipschitz continuous on $\mathbb{R}^n$. Further assume that $f(x)$ is bounded from below on $\mathbb{R}^n$. Let $\{x_k\}$ be the iterates generated by the modified/quasi-Newton Wolfe lineasearch Algorithms 16 or 17, such that B_k has uniformly bounded condition number. Then there exists a constant M such that for all $T \geq 1$

$$\min_{k=0,\ldots,T} \|\nabla f(x_k)\| \leq \frac{M}{\sqrt{T+1}}.$$

Consequently, for any $\epsilon > 0$, within $\lceil (\frac{M}{\epsilon})^2 \rceil$ steps, we will see an iterate where the gradient has norm at most ϵ. In other words, we reach an "ϵ-stationary" point in $O((\frac{1}{\epsilon})^2)$ steps

Notes

Rate of convergence

Theorem 4.9 (Local superlinear convergence for quasi-Newton)

Suppose that

- *$f \in \mathcal{C}^2$*
- *H is Lipschitz continuous on $\mathbb{R}^n$*

Suppose that iterates are generated from the quasi-Newton Wolfe Algorithm Algorithm 17 such that $0 < c_1 < c_2 \leq \frac{1}{2}$.

If the sequence of iterates $\{x_k\}$ has a limit point x^* satisfying $H(x^*)$ is positive definite and $g(x^*) = 0$, then it follows that

(i) *the step length $\alpha_k = 1$ is valid for all sufficiently large k,*
(ii) *the entire sequence $\{x_k\}$ converges to x^* superlinearly.*

See also Theorems 3.6 and 3.7 from Nocedal-Wright.

Notes

A Summary

The problem

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x)$$

where the objective function $f : \mathbb{R}^n \to \mathbb{R}$

Solve instead quadratic approximation at current iterate x_k, after choosing positive definite B_k, to get a search direction that is a descent direction:

$$p_k = \underset{p \in \mathbb{R}^n}{\text{argmin}} \; m_k^Q(p) \stackrel{\text{def}}{=} f_k + g_k^T p + \frac{1}{2} p^T B_k p$$

- B_k = identity matrix: Steepest Descent Direction.
- B_k obtained from Hessian H_k by adjusting eigenvalues: Modified-Newton.
- B_k obtained by updating at every iteration using current and previous gradient information: Quasi-Newton.

Decide on step size strategy: Armijo backtracking line search, Wolfe backtracking line search, constant step size (HW assignment), $O\left(\frac{1}{\sqrt{k}}\right)$ in iteration k ... many others.

Notes

A Summary

Steepest Descent	Modified/Quasi Newton
Requires only function and gradient evaluations	Could need Hessian evaluations as well (with spectral decompositions)
No overhead of solving linear system in each iteration	Solves a linear system Bp = g in each iteration
Global convergence to ϵ-stationary point in $O((\frac{1}{\epsilon})^2)$ steps	Global convergence to ϵ-stationary point in $O((\frac{1}{\epsilon})^2)$ steps
Linear local convergence: converges to ϵ distance from local minimum in $O(\log(\frac{1}{\epsilon}))$ steps	Superlinear (quadratic) local convergence: converges to ϵ distance from local minimum in $o(\log(\frac{1}{\epsilon}))$ ($O(\log\log(\frac{1}{\epsilon}))$ steps.

Notes