# Part 2: Linesearch methods for unconstrained optimization

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

Part C course on continuoue optimization

## UNCONSTRAINED MINIMIZATION

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

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

- assume that $f \in C^1$ (sometimes $C^2$) and Lipschitz
- often in practice this assumption violated, but not necessary

## ITERATIVE METHODS

- in practice very rare to be able to provide explicit minimizer
- iterative method: given starting "guess" $x_0$, generate sequence

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

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

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

## LINESEARCH METHODS

- calculate a **search direction** $p_k$ from $x_k$
- ensure that this direction is a **descent direction**, i.e.,

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

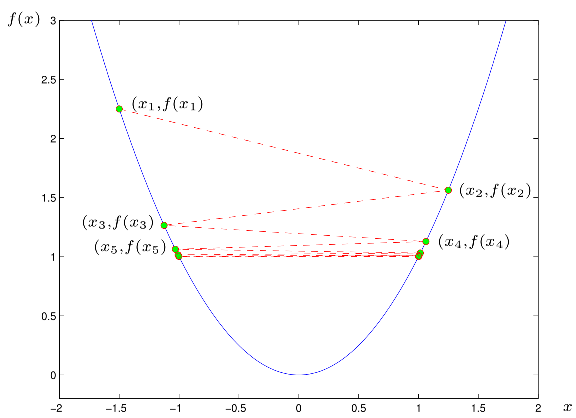
  so that, for small steps along $p_k$, the objective function **will** be reduced
- calculate a suitable **steplength** $\alpha_k > 0$ so that

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

- computation of $\alpha_k$ is the **linesearch**—may itself be an iteration
- generic linesearch method:

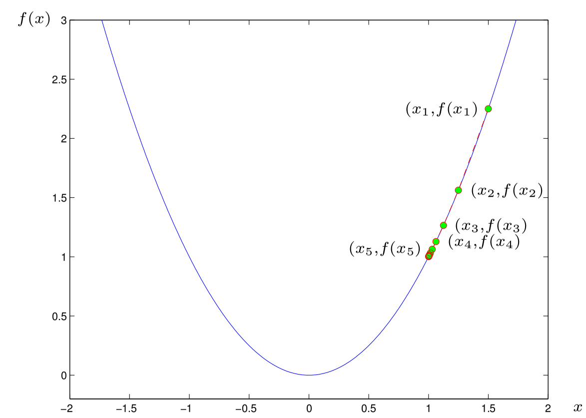
$$x_{k+1} = x_k + \alpha_k p_k$$

## STEPS MIGHT BE TOO LONG




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 $x_0 = 2$

## STEPS MIGHT BE TOO SHORT




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 $x_0 = 2$

## PRACTICAL LINESEARCH METHODS

- in early days, pick $\alpha_k$ to minimize

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

  - **exact** linesearch—univariate minimization
  - rather expensive and certainly not cost effective
- modern methods: **inexact** linesearch
  - ensure steps are neither too long nor too short
  - try to pick "useful" initial stepsize for fast convergence
  - best methods are either
    - "backtracking- Armijo" or
    - "Armijo-Goldstein"

  based

## BACKTRACKING LINESEARCH

Procedure to find the stepsize $\alpha_k$:

> Given $\alpha_{\text{init}} > 0$ (e.g., $\alpha_{\text{init}} = 1$)
> let $\alpha^{(0)} = \alpha_{\text{init}}$ and $l = 0$
> Until $f(x_k + \alpha^{(l)} p_k)$ "<" $f_k$
> set $\alpha^{(l+1)} = \tau\alpha^{(l)}$, where $\tau \in (0, 1)$ (e.g., $\tau = \frac{1}{2}$)
> and increase $l$ by 1
> Set $\alpha_k = \alpha^{(l)}$

- this prevents the step from getting too small . . . but does not prevent too large steps relative to decrease in $f$
- need to tighten requirement

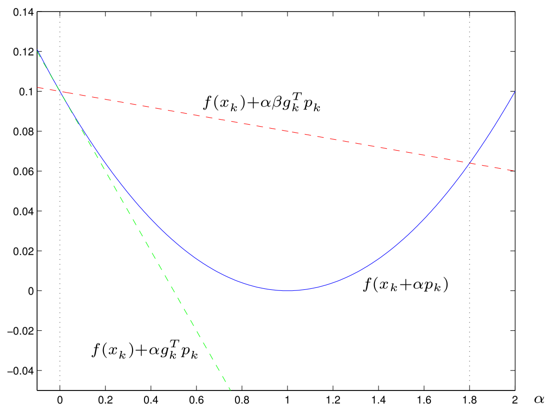
$$f(x_k + \alpha^{(l)} p_k) \text{“}<\text{”} f_k$$

## ARMIJO CONDITION

In order to prevent large steps relative to decrease in $f$, instead require

$$f(x_k + \alpha_k p_k) \le f(x_k) + \alpha_k \beta g_k^T p_k$$

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




## BACKTRACKING-ARMIJO LINESEARCH

Procedure to find the stepsize $\alpha_k$:

> Given $\alpha_{\text{init}} > 0$ (e.g., $\alpha_{\text{init}} = 1$)
> let $\alpha^{(0)} = \alpha_{\text{init}}$ and $l = 0$
> Until $f(x_k + \alpha^{(l)} p_k) \le f(x_k) + \alpha^{(l)} \beta g_k^T p_k$
> set $\alpha^{(l+1)} = \tau \alpha^{(l)}$, where $\tau \in (0,1)$ (e.g., $\tau = \frac{1}{2}$)
> and increase $l$ by 1
> Set $\alpha_k = \alpha^{(l)}$

## SATISFYING THE ARMIJO CONDITION

> **Theorem 2.1.** Suppose that $f \in C^1$, that $g(x)$ is Lipschitz continuous with Lipschitz constant $\gamma(x)$, that $\beta \in (0,1)$ and that $p$ is a descent direction at $x$. Then the Armijo condition
>
> $$f(x + \alpha p) \le f(x) + \alpha \beta g(x)^T p$$
>
> is satisfied for all $\alpha \in [0, \alpha_{\max(x)}]$, where
>
> $$\alpha_{\max} = \frac{2(\beta - 1) g(x)^T p}{\gamma(x) \|p\|_2^2}$$

## PROOF OF THEOREM 2.1

Taylor's theorem (Theorem 1.1) +

$$\alpha \le \frac{2(\beta - 1) g(x)^T p}{\gamma(x) \|p\|_2^2},$$

$\Longrightarrow$

$$\begin{aligned} f(x + \alpha p) &\le f(x) + \alpha g(x)^T p + \tfrac{1}{2}\gamma(x)\alpha^2 \|p\|^2 \\ &\le f(x) + \alpha g(x)^T p + \alpha(\beta - 1) g(x)^T p \\ &= f(x) + \alpha \beta g(x)^T p \end{aligned}$$

## THE ARMIJO LINESEARCH TERMINATES

**Corollary 2.2.** Suppose that $f \in C^1$, that $g(x)$ is Lipschitz continuous with Lipschitz constant $\gamma_k$ at $x_k$, that $\beta \in (0,1)$ and that $p_k$ is a descent direction at $x_k$. Then the stepsize generated by the backtracking-Armijo linesearch terminates with

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

## PROOF OF COROLLARY 2.2

Theorem 2.1 $\Longrightarrow$ linesearch will terminate as soon as $\alpha^{(l)} \leq \alpha_{\max}$.

2 cases to consider:

1. May be that $\alpha_{\text{init}}$ satisfies the Armijo condition $\Longrightarrow \alpha_k = \alpha_{\text{init}}$.
2. Otherwise, must be a last linesearch iteration (the $l$-th) for which

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

Combining these 2 cases gives required result.

## GENERIC LINESEARCH METHOD

Given an initial guess $x_0$, let $k = 0$
Until convergence:
  Find a descent direction $p_k$ at $x_k$
  Compute a stepsize $\alpha_k$ using a
    backtracking-Armijo linesearch along $p_k$
  Set $x_{k+1} = x_k + \alpha_k p_k$, and increase $k$ by 1

## GLOBAL CONVERGENCE THEOREM

**Theorem 2.3.** Suppose that $f \in C^1$ and that $g$ is Lipschitz continuous on $\mathbb{R}^n$. Then, for the iterates generated by the Generic Linesearch Method,

either

$$g_l = 0 \text{ for some } l \geq 0$$

or

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

or

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

## PROOF OF THEOREM 2.3

Suppose that $g_k \neq 0$ for all $k$ and that $\lim_{k\to\infty} f_k > -\infty$. Armijo $\Longrightarrow$

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

for all $k \Longrightarrow$ summing over first j iterations

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

LHS bounded below by assumption $\Longrightarrow$ RHS bounded below. Sum composed of -ve terms $\Longrightarrow$

$$\lim_{k\to\infty} \alpha_k |p_k^T g_k| = 0$$

Let

$$\mathcal{K}_1 \stackrel{\text{def}}{=} \left\{ k \mid \alpha_{\text{init}} > \frac{2\tau(\beta-1)g_k^T p_k}{\gamma \|p_k\|_2^2} \right\} \;\; \& \;\; \mathcal{K}_2 \stackrel{\text{def}}{=} \{1,2,\ldots\} \setminus \mathcal{K}_1$$

where $\gamma$ is the assumed uniform Lipschitz constant.

For $k \in \mathcal{K}_1$,

$$\alpha_k \geq \frac{2\tau(\beta-1)g_k^T p_k}{\gamma \|p_k\|_2^2}$$

$\Longrightarrow$

$$\alpha_k p_k^T g_k \leq \frac{2\tau(\beta-1)}{\gamma} \left( \frac{g_k^T p_k}{\|p_k\|} \right)^2 < 0$$

$\Longrightarrow$

$$\lim_{k\in\mathcal{K}_1\to\infty} \frac{|p_k^T g_k|}{\|p_k\|_2} = 0. \tag{1}$$

For $k \in \mathcal{K}_2$,

$$\alpha_k \geq \alpha_{\text{init}}$$

$\Longrightarrow$

$$\lim_{k\in\mathcal{K}_2\to\infty} |p_k^T g_k| = 0. \tag{2}$$

Combining (1) and (2) gives the required result.

## METHOD OF STEEPEST DESCENT

The search direction

$$p_k = -g_k$$

gives the so-called **steepest-descent** direction.

- $p_k$ is a descent direction
- $p_k$ solves the problem

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

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

## GLOBAL CONVERGENCE FOR STEEPEST DESCENT

**Theorem 2.4.** Suppose that $f \in C^1$ and that $g$ is Lipschitz continuous on $\mathbb{R}^n$. Then, for the iterates generated by the Generic Linesearch Method using the steepest-descent direction,

either

$$g_l = 0 \;\; \text{for some} \;\; l \geq 0$$

or

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

or

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

## PROOF OF THEOREM 2.4

Follows immediately from Theorem 2.3, since

$$\min\left(|p_k^T g_k|, |p_k^T g_k|/\|p_k\|_2\right) = \|g_k\|_2 \min\left(1, \|g_k\|_2\right)$$

and thus

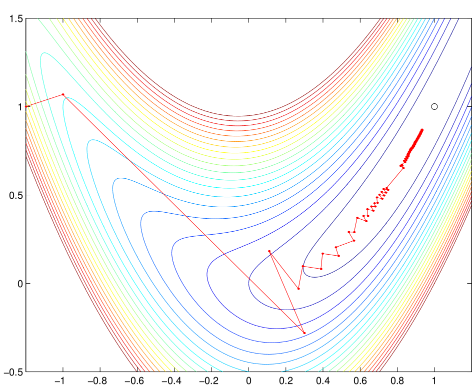
$$\lim_{k\to\infty} \min\left(|p_k^T g_k|, |p_k^T g_k|/\|p_k\|_2\right) = 0$$

implies that $\lim_{k\to\infty} g_k = 0$.

## METHOD OF STEEPEST DESCENT (cont.)

- archetypical globally convergent method
- many other methods resort to steepest descent in bad cases
- not scale invariant
- convergence is usually very (very!) slow (linear)
- numerically often not convergent at all

## STEEPEST DESCENT EXAMPLE




Contours for the objective function $f(x,y) = 10(y-x^2)^2 + (x-1)^2$, and the iterates generated by the Generic Linesearch steepest-descent method

## MORE GENERAL DESCENT METHODS

Let $B_k$ be a symmetric, positive definite matrix, and define the search direction $p_k$ so that

$$B_k p_k = -g_k$$

Then

- $p_k$ is a descent direction
- $p_k$ solves the problem

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

- if the Hessian $H_k$ is positive definite, and $B_k = H_k$, this is **Newton's method**

## MORE GENERAL GLOBAL CONVERGENCE

**Theorem 2.5.** Suppose that $f \in C^1$ and that $g$ is Lipschitz continuous on $\mathbb{R}^n$. Then, for the iterates generated by the Generic Linesearch Method using the more general descent direction, either

$$g_l = 0 \text{ for some } l \geq 0$$

or

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

or

$$\lim_{k\to\infty} g_k = 0$$

provided that the eigenvalues of $B_k$ are uniformly bounded and bounded away from zero.

$\Longrightarrow$

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

Thus

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

$\Longrightarrow$

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

$\Longrightarrow$

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

## PROOF OF THEOREM 2.5

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

$$\lambda_{\min} \leq \lambda_{\min}(B_k) \leq \frac{s^T B_k s}{\|s\|^2} \leq \lambda_{\max}(B_k) \leq \lambda_{\max}$$

and thus that

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

for any nonzero vector $s$. Thus

$$|p_k^T g_k| = |g_k^T B_k^{-1} g_k| \geq \lambda_{\min}(B_k^{-1})\|g_k\|_2^2 \geq \lambda_{\max}^{-1}\|g_k\|_2^2$$

In addition

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

$\Longrightarrow$

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

## MORE GENERAL DESCENT METHODS (cont.)

- ⊙ may be viewed as "scaled" steepest descent
- ⊙ convergence is often faster than steepest descent
- ⊙ can be made scale invariant for suitable $B_k$

## CONVERGENCE OF NEWTON'S METHOD

**Theorem 2.6.** Suppose that $f \in C^2$ and that $H$ is Lipschitz continuous on $\mathbb{R}^n$. Then suppose that the iterates generated by the Generic Linesearch Method with $\alpha_{\text{init}} = 1$ and $\beta < \frac{1}{2}$, in which the search direction is chosen to be the Newton direction $p_k = -H_k^{-1} g_k$ whenever possible, has a limit point $x_*$ for which $H(x_*)$ is positive definite. Then

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

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

(iii) the rate is Q-quadratic, i.e, there is a constant $\kappa \geq 0$.

$$\lim_{k \to \infty} \frac{\|x_{k+1} - x_*\|_2}{\|x_k - x_*\|_2^2} \leq \kappa.$$

Taylor's theorem $\Longrightarrow$ $\exists z_k$ 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 $H$ & $H_k p_k + g_k = 0 \Longrightarrow$

$$\begin{aligned} f(x_k + p_k) - f_k - \tfrac{1}{2} p_k^T g_k &= \tfrac{1}{2}(p_k^T g_k + p_k^T H(z_k) p_k) \\ &= \tfrac{1}{2}(p_k^T g_k + p_k^T H_k p_k) + \tfrac{1}{2}(p_k^T (H(z_k) - H_k) p_k) \\ &\leq \tfrac{1}{2}\gamma \|z_k - x_k\|_2 \|p_k\|_2^2 \leq \tfrac{1}{2}\gamma \|p_k\|_2^3 \end{aligned} \tag{4}$$

Now pick $k$ sufficiently large so that

$$\gamma \|p_k\|_2 \leq \lambda_{\min}(H_*)(1 - 2\beta).$$

+ (3) + (4) $\Longrightarrow$

$$\begin{aligned} f(x_k + p_k) - f_k &\leq \tfrac{1}{2} p_k^T g_k + \tfrac{1}{2}\lambda_{\min}(H_*)(1 - 2\beta)\|p_k\|_2^2 \\ &\leq \tfrac{1}{2}(1 - (1 - 2\beta)) p_k^T g_k = \beta p_k^T g_k \end{aligned}$$

$\Longrightarrow$ unit stepsize satisfies the Armijo condition for all sufficiently large $k \in \mathcal{K}$

## PROOF OF THEOREM 2.6

Consider $\lim_{k \in \mathcal{K}} x_k = x_*$. Continuity $\Longrightarrow$ $H_k$ positive definite for all $k \in \mathcal{K}$ sufficiently large $\Longrightarrow$ $\exists k_0 \geq 0$:

$$p_k^T H_k p_k \geq \tfrac{1}{2}\lambda_{\min}(H_*)\|p_k\|_2^2$$

$\forall k_0 \leq k \in \mathcal{K}$, where $\lambda_{\min}(H_*)$ = smallest eigenvalue of $H(x_*)$ $\Longrightarrow$

$$|p_k^T g_k| = -p_k^T g_k = p_k^T H_k p_k \geq \tfrac{1}{2}\lambda_{\min}(H_*)\|p_k\|_2^2. \tag{3}$$

$\forall k_0 \leq k \in \mathcal{K}$, and

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

since Theorem 2.5 $\Longrightarrow$ at least one of the LHS of (3) and

$$\frac{|p_k^T g_k|}{\|p_k\|_2} = -\frac{p_k^T g_k}{\|p_k\|_2} \geq \tfrac{1}{2}\lambda_{\min}(H_*)\|p_k\|_2$$

converges to zero for such $k$.

Now note that $\|H_k^{-1}\|_2 \leq 2/\lambda_{\min}(H_*)$ for all sufficiently large $k \in \mathcal{K}$. The iteration gives

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

But Theorem 1.3 $\Longrightarrow$

$$\|g(x_*) - g_k - H_k(x_* - x_k)\|_2 \leq \gamma \|x_* - x_k\|_2^2$$

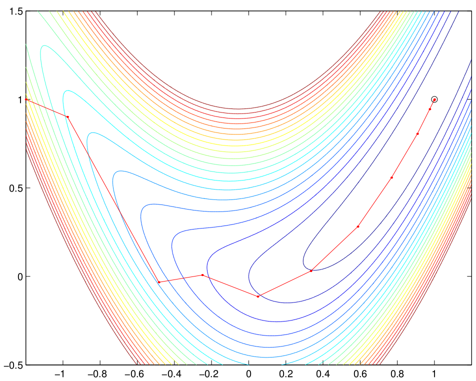
$\Longrightarrow$

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

which is (iii) when $\kappa = 2\gamma/\lambda_{\min}(H_*)$. for $k \in \mathcal{K}$.

Result (ii) follows since once iterate becomes sufficiently close to $x_*$, (iii) for $k \in \mathcal{K}$ sufficiently large implies $k + 1 \in \mathcal{K} \Longrightarrow \mathcal{K} = \mathbb{N}$. Thus (i) and (iii) are true for all $k$ sufficiently large.

## NEWTON METHOD EXAMPLE




Contours for the objective function $f(x,y) = 10(y - x^2)^2 + (x-1)^2$, and the iterates generated by the Generic Linesearch Newton method

## QUASI-NEWTON METHODS

Various attempts to approximate $H_k$:

- Finite-difference approximations:

$$(H_k)e_i \approx h^{-1}(g(x_k + he_i) - g_k) = (B_k)e_i$$

  for some "small" scalar $h > 0$

- Secant approximations: try to ensure the **secant condition**

  $B_{k+1}s_k = y_k \approx H_{k+1}s_k$, where $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$

  - **Symmetric Rank-1 method** (but may be indefinite or even fail):

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

  - **BFGS method**: (symmetric and positive definite if $y_k^T s_k > 0$):

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

## MODIFIED NEWTON METHODS

If $H_k$ is indefinite, it is usual to solve instead

$$(H_k + M_k)p_k \equiv B_k p_k = -g_k$$

where

- $M_k$ chosen so that $B_k = H_k + M_k$ is "sufficiently" positive definite
- $M_k = 0$ when $H_k$ is itself "sufficiently" positive definite

Possibilities:

- If $H_k$ has the spectral decomposition $H_k = Q_k D_k Q_k^T$ then

$$B_k \equiv H_k + M_k = Q_k \max(\epsilon, |D_k|) Q_k^T$$

- $M_k = \max(0, \epsilon - \lambda_{\min}(H_k))I$
- **Modified Cholesky**: $B_k \equiv H_k + M_k = L_k L_k^T$

## MINIMIZING A CONVEX QUADRATIC MODEL

For convex models ($B_k$ positive definite)

$$p_k = \text{(approximate)} \arg\min_{p \in \mathbb{R}^n} f_k + p^T g_k^T + \tfrac{1}{2} p^T B_k p$$

**Generic convex quadratic problem:** ($B$ positive definite)

$$\text{(approximately) minimize}_{p \in \mathbb{R}^n} \; q(p) = p^T g + \tfrac{1}{2} p^T B p$$

## MINIMIZATION OVER A SUBSPACE

Given vectors $\{d^0, : \ldots, d^{i-1}\}$, let

- $\odot$ $D^i = (d^0 : \cdots : d^{i-1})$
- $\odot$ Subspace $\mathcal{D}^i = \{p \mid p = D^i p_d \;\text{ for some }\; p_d \in \mathbb{R}^i\}$
- $\odot$ $p^i = \underset{p \in \mathcal{D}^i}{\arg\min}\; q(p)$

**Result**: $D^{i\,T} g^i = 0$, where $g^i = Bp^i + g$
**Proof**: require $p^i = D^i p_d^i$, where $p_d^i = \underset{p_d \in \mathbb{R}^i}{\arg\min}\; q(D^i p_d)$
But $q(D^i p_d) = p_d^T D^{i\,T} g + \frac{1}{2} p_d^T D^{i\,T} B D^i p_d \Longrightarrow$
$0 = D^{i\,T} B D^i p_d^i + D^{i\,T} g = D^{i\,T}(BD^i p_d^i + g) = D^{i\,T}(Bp^i + g) = D^{i\,T} g^i$

**Equivalently**: $d^{j\,T} g^i = 0$ for $j = 0, \ldots, i-1$

## MINIMIZATION OVER A SUBSPACE (cont.)

- $\odot$ $d^{j\,T} g^i = 0$ for $j = 0, \ldots, i-1$, where $g^i = Bp^i + g$

**Result**: $p^i = p^{i-1} - d^{i-1\,T} g^{i-1} D^i (D^{i\,T} B D^i)^{-1} e_i$

**Proof**: Clearly $p^{i-1} \in \mathcal{D}^{i-1} \subset \mathcal{D}^i$
$\Longrightarrow$ require $p^i = p^{i-1} + D^i p_d^i$, where $p_d^i = \underset{p_d \in \mathbb{R}^i}{\arg\min}\; q(p^{i-1} + D^i p_d)$
But $q(p^{i-1} + D^i p_d)$
$= q(p^{i-1}) + p_d^T D^{i\,T}(g + Bp^{i-1}) + \frac{1}{2} p_d^T D^{i\,T} B D^i p_d$
$= q(p^{i-1}) + p_d^T D^{i\,T} g^{i-1} + \frac{1}{2} p_d^T D^{i\,T} B D^i p_d$
$= q(p^{i-1}) + p_d^T (d^{i-1\,T} g^{i-1}) e_i + \frac{1}{2} p_d^T D^{i\,T} B D^i p_d$
where $e_i$ is $i$-th unit vector $\Longrightarrow$
$p_d^i = -d^{i-1\,T} g^{i-1} (D^{i\,T} B D^i)^{-1} e_i$

## MINIMIZATION OVER A B-CONJUGATE SUBSPACE

Minimizer over $\mathcal{D}^i$: $p^i = p^{i-1} - d^{i-1\,T} g^{i-1} D^i (D^{i\,T} B D^i)^{-1} e_i$

Suppose in addition the members of $\mathcal{D}^i$ are $B$-conjugate:

- $\odot$ **B-conjugacy**: $d^{i\,T} B d^j = 0 \; (i \neq j)$

**Result**: $p^i = p^{i-1} + \alpha^{i-1} d^{i-1}$, where

$$\alpha^{i-1} = -\frac{d^{i-1\,T} g^{i-1}}{d^{i-1\,T} B d^{i-1}}$$

**Proof**: $D^{i\,T} B D^i =$ diagonal matrix with entries $d^{j\,T} B d^j$
for $j = 0, \ldots i-1$
$\Longrightarrow$ $(D^{i\,T} B D^i)^{-1} =$ diagonal matrix with entries $1/d^{j\,T} B d^j$
for $j = 0, \ldots i-1$
$\Longrightarrow$ $(D^{i\,T} B D^i)^{-1} e_i = (1/d^{i-1\,T} B d^{i-1}) e_i$

## BUILDING A B-CONJUGATE SUBSPACE

- $\odot$ $d^{j\,T} g^i = 0$ for $j = 0, \ldots, i-1$

Since this implies $g^i$ is independent of $\mathcal{D}^i$, let

$$d^i = -g^i + \sum_{j=0}^{i-1} \beta^{ij} d^j$$

**Aim**: find $\beta^{ij}$ so that $d^i$ is $B$-conjugate to $\mathcal{D}^i$

**Result** (orthogonal gradients): $g^{i\,T} g^j = 0$ for all $i \neq j$
**Proof**: $\text{span}\{g^i\} = \text{span}\{d^i\}$
$\Longrightarrow$ $g^j = \sum_{k=0}^{j} \gamma^{j,k} d^k$ for some $\gamma^{j,k}$
$\Longrightarrow$ $g^{i\,T} g^j = \sum_{k=0}^{j} \gamma^{j,k} g^{i\,T} d^k = 0$ when $j < i$

## BUILDING A B-CONJUGATE SUBSPACE (cont.)

- $d^i = -g^i + \sum_{j=0}^{i-1} \beta^{ij} d^j$
- ${d^j}^T g^i = 0$ for $j = 0, \ldots, i-1$, where $g^i = Bp^i + g$

**Result**: ${g^i}^T d^i = -\|g^i\|_2^2$
**Proof**: ${g^i}^T d^i = -{g^i}^T g^i + \sum_{j=0}^{i-1} \beta^{ij} {g^i}^T d^j$

**Corollary**: $\alpha^i = \dfrac{\|g^i\|_2^2}{{d^i}^T B d^i} \neq 0 \Longleftrightarrow g^i \neq 0$

**Proof**: by definition

$$\alpha^i = -\frac{{g^i}^T d^i}{{d^i}^T B d^i}$$

## BUILDING A B-CONJUGATE SUBSPACE (cont.)

- $d^i = -g^i + \sum_{j=0}^{i-1} \beta^{ij} d^j$
- ${g^i}^T g^j = 0$ for all $i \neq j$

**Result**: ${g^i}^T B d^j = 0$ if $j < i-1$ and ${g^i}^T B d^{i-1} = \dfrac{\|g^i\|_2^2}{\alpha^{i-1}}$

**Proof**: $p^{j+1} = p^j + \alpha^j d^j$ & $g^{j+1} = Bp^{j+1} + g$
$\Longrightarrow g^{j+1} = g^j + \alpha^j B d^j$
$\Longrightarrow {g^i}^T g^{j+1} = {g^i}^T g^j + \alpha^j {g^i}^T B d^j$
$\Longrightarrow {g^i}^T B d^j = 0$ if $j < i-1$
while ${g^i}^T g^i = {g^i}^T g^{i-1} + \alpha^{i-1} {g^i}^T B d^{i-1}$ if $j = i-1$
$\Longrightarrow {g^i}^T B d^{i-1} = \|g^i\|_2^2 / \alpha^{i-1}$

## BUILDING A B-CONJUGATE SUBSPACE (cont.)

- $d^i = -g^i + \sum_{k=0}^{i-1} \beta^{ik} d^k$
- ${d^k}^T B g^i = 0$ if $k < i-1$ and ${d^{i-1}}^T B g^i = \|g^i\|_2^2 / \alpha^{i-1}$
- $\alpha^{i-1} = \|g^{i-1}\|_2^2 / {d^{i-1}}^T B d^{i-1}$

**Result**: $\beta^{ij} = 0$ for $j < i-1$ and $\beta^{i\,i-1} \equiv \beta^i = \dfrac{\|g_i\|_2^2}{\|g_{i-1}\|_2^2}$

**Proof**: B-conjugacy $\Longrightarrow$

$$0 = {d^j}^T B d^i = -{d^j}^T B g^i + \sum_{k=0}^{i-1} \beta^{ik} {d^j}^T B d^k = -{d^j}^T B g^i + \beta^{ij} {d^j}^T B d^j$$

$\Longrightarrow \beta^{ij} = {d^j}^T B g^i / {d^j}^T B d^j$
Result immediate for $j < i-1$. For $j = i-1$,

$$\beta^{i\,i-1} = \frac{{d^{i-1}}^T B g^i}{{d^{i-1}}^T B d^{i-1}} = \frac{\|g^i\|_2^2}{\alpha^{i-1} {d^{i-1}}^T B d^{i-1}} = \frac{\|g^i\|_2^2}{\|g^{i-1}\|_2^2}$$

## CONJUGATE-GRADIENT METHOD

> Given $p^0 = 0$, set $g^0 = g$, $d^0 = -g$ and $i = 0$.
> Until $g^i$ "small" iterate
> $\alpha^i = -{g^i}^T d^i / {d^i}^T B d^i$
> $p^{i+1} = p^i + \alpha^i d^i$
> $g^{i+1} = g^i + \alpha^i B d^i$
> $\beta^i = \|g^{i+1}\|_2^2 / \|g^i\|_2^2$
> $d^{i+1} = -g^{i+1} + \beta^i d^i$
> and increase $i$ by 1

Important features

- ${d^j}^T g^{i+1} = 0 = {g^j}^T g^{i+1}$ for all $j = 0, \ldots, i$
- $g^T p^i < 0$ for $i = 1, \ldots, n \Longrightarrow$ descent direction for any $p_k = p^i$
- **stop**: $\|g^i\| \leq \min(\|g\|^\omega, \eta)\|g\|$ $(0 < \eta, \omega < 1) \Longrightarrow$ fast convergence

## CONJUGATE GRADIENT METHOD GIVES DESCENT

$$g^{i-1\,T}d^{i-1} = d^{i-1\,T}(g + Bp^{i-1}) = d^{i-1\,T}g + \sum_{j=0}^{i-2}\alpha_j d^{i-1\,T}Bd^j = d^{i-1\,T}g$$

$p^i$ minimizes $q(p)$ in $\mathcal{D}^i \Longrightarrow$

$$p^i = p^{i-1} - \frac{g^{i-1\,T}d^{i-1}}{d^{i-1\,T}Bd^{i-1}}d^{i-1} = p^{i-1} - \frac{g^Td^{i-1}}{d^{i-1\,T}Bd^{i-1}}d^{i-1}.$$

$\Longrightarrow$

$$g^Tp^i = g^Tp^{i-1} - \frac{(g^Td^{i-1})^2}{d^{i-1\,T}Bd^{i-1}},$$

$\Longrightarrow$ $g^Tp^i < g^Tp^{i-1} \Longrightarrow$ (induction)

$$g^Tp^i < 0$$

since

$$g^Tp^1 = -\frac{\|g\|_2^4}{g^TBg} < 0.$$

$\Longrightarrow$ $p_k = p^i$ is a descent direction

## NONLINEAR CONJUGATE-GRADIENT METHODS

method for minimizing quadratic $f(x)$

Given $x^0$ and $g(x_0)$, set $d^0 = -g(x_0)$ and $i = 0$.
Until $g(x_k)$ "small" iterate
  $\alpha^i = \arg\min_\alpha f(x_i + \alpha d^i)$
  $x_{i+1} = x_i + \alpha^i d^i$
  $\beta^i = \|g(x_{i+1})\|_2^2 / \|g(x_i)\|_2^2$
  $d^{i+1} = -g(x_{i+1}) + \beta^i d^i$
  and increase $i$ by 1

may also be used for nonlinear $f(x)$ (Fletcher & Reeves)

- replace calculation of $\alpha^i$ by suitable linesearch
- other methods pick different $\beta^i$ to ensure descent

## CG METHODS FOR GENERAL QUADRATICS

Suppose $f(x)$ is quadratic and $x = x_0 + p$
Taylors theorem $\Longrightarrow$

$$f(x) = f(x_0 + p) = f(x_0) + p^Tg(x_0) + \tfrac{1}{2}p^TH(x_0)p$$

- can minimize as function of $p$ using CG
- if $x_i = x_0 + p_i \Longrightarrow g^i = g(x_0) + H(x_0)p_i = g(x_i)$
- $\alpha^i = -\dfrac{g(x_i)^Td^i}{d^{i\,T}H(x_0)d^i} = \arg\min_\alpha f(x_i + \alpha d^i)$