

# Part 2: Linesearch methods for unconstrained optimization

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

MSc course on nonlinear optimization

# UNCONSTRAINED MINIMIZATION

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

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

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

- ◉ **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

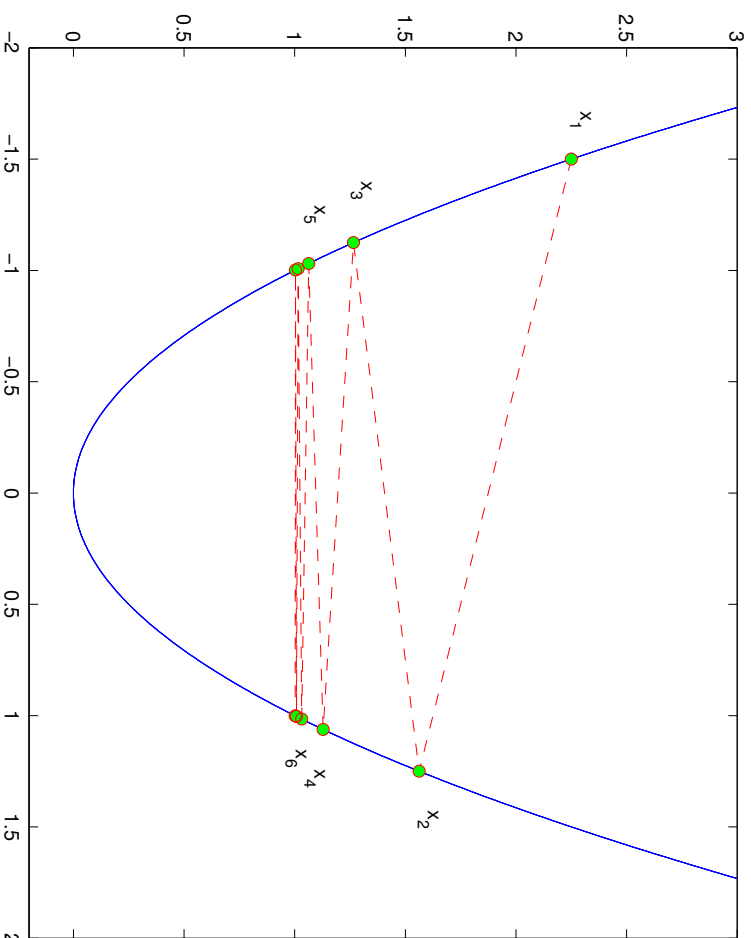
- ◉ calculate a suitable **steplength**  $\alpha_k > 0$  so that

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

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

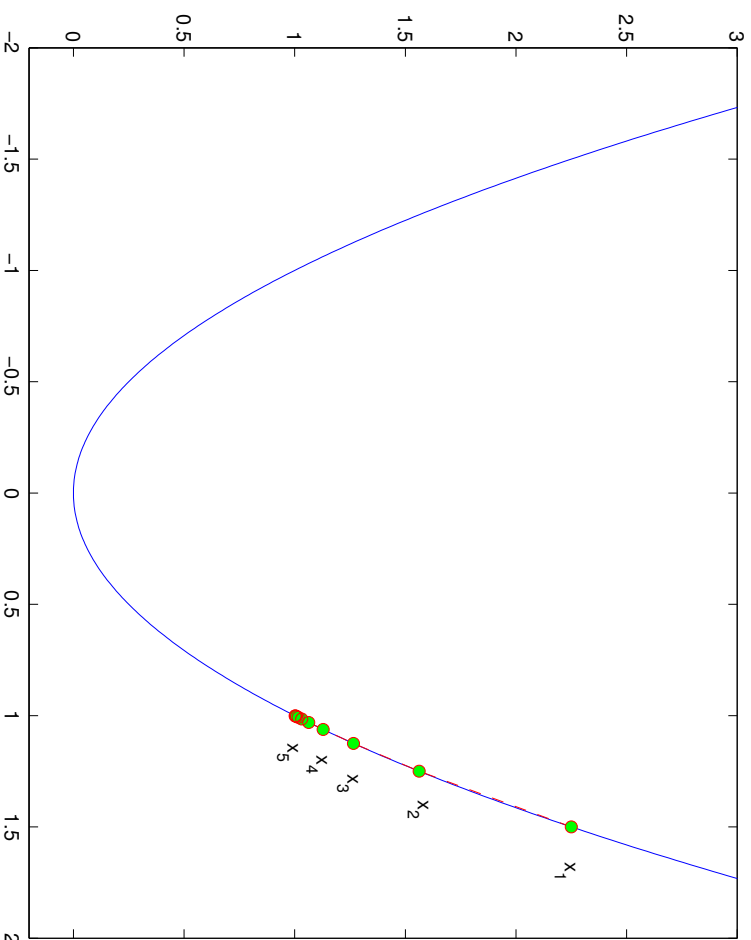
$$x_{k+1} = x_k + \alpha_k p_k$$

## 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  $f(x_k + \alpha^{(l)} p_k) \leq f_k$   
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

$$f(x_k + \alpha^{(l)} p_k) \leq f_k$$

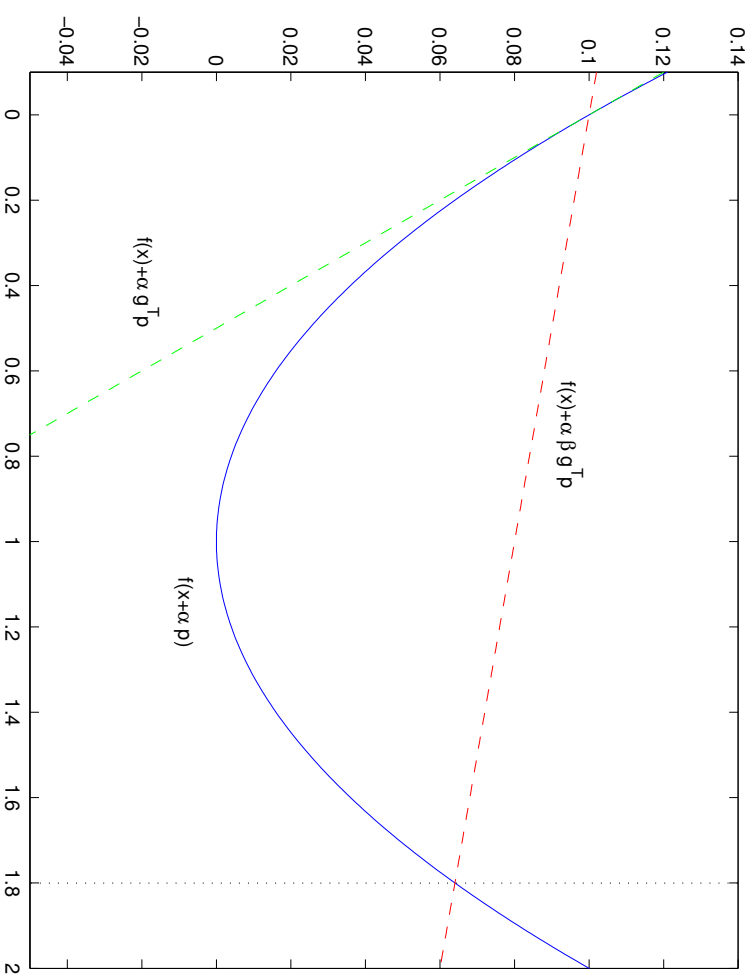


## ARMJO CONDITION

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

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

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



## BACKTRACKING-ARMJO 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  $f(x_k + \alpha^{(l)}p_k) \leq f(x_k) + \alpha^{(l)}\beta g_k^T p_k$   
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

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

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) +

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

$\implies$

$$\begin{aligned} f(x + \alpha p) &\leq f(x) + \alpha g(x)^T p + \frac{1}{2} \gamma(x) \alpha^2 \|p\|_2^2 \\ &\leq f(x) + \alpha g(x)^T p + \alpha(\beta - 1)g(x)^T p \\ &= f(x) + \alpha \beta g(x)^T p \end{aligned}$$

## 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  $\implies$  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  $\implies \alpha_k = \alpha_{\text{init}}$ .
2. Otherwise, must be a last linesearch iteration (the  $l$ -th) for which

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

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

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

or

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



## PROOF OF THEOREM 2.3

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

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

for all  $k \implies$  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  $\implies$  RHS bounded below. Sum composed of -ve terms  $\implies$

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

Let

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

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

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

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

$\implies$

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

$\implies$

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

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

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

$\implies$

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

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

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

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

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

or

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

## PROOF OF THEOREM 2.4

Follows immediately from Theorem 2.3, since

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

and thus

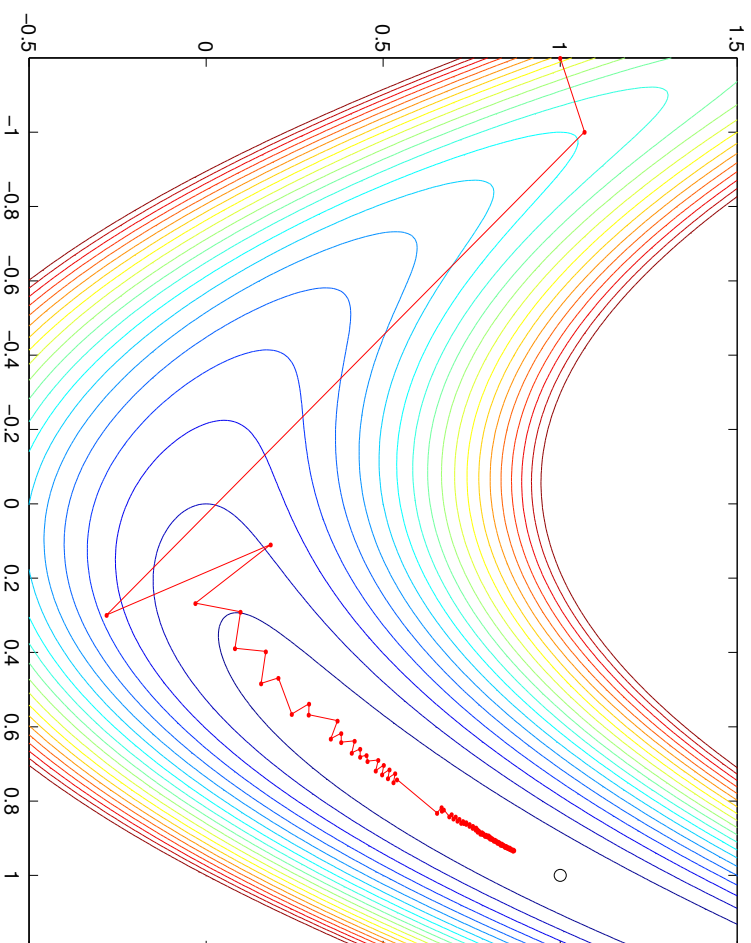
$$\lim_{k \rightarrow \infty} \min (|p_k^T g_k|, |p_k^T g_k|/\|p_k\|_2) = 0$$

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

## 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

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

- 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

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

or

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

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

## 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

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

In addition

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

$\implies$

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

$\implies$ 

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

Thus

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

 $\implies$ 

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

 $\implies$ 

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

## 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  $\kappa \geq 0$ .

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

## PROOF OF THEOREM 2.6

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

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

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

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

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

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

since Theorem 2.5  $\implies$  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  $k$ .

Taylor's theorem  $\implies \exists z_k$  between  $x_k$  and  $x_k + p_k$  such that

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

Lipschitz continuity of  $H$  &  $H_k p_k + g_k = 0 \implies$

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

Now pick  $k$  sufficiently large so that

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

+ (3) + (4)  $\implies$

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

$\implies$  unit stepsize satisfies the Armijo condition, which proves (i).

To obtain the remaining results, 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  $\implies$

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

$\implies$

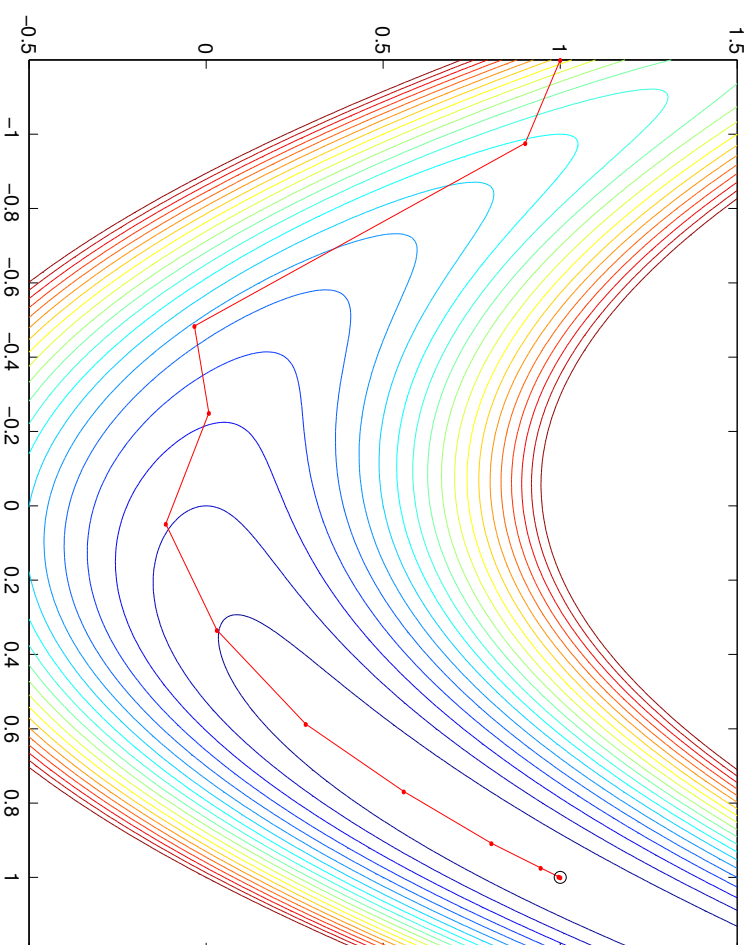
$$\|x_{k+1} - x_*\|_2 \leq \gamma \|H_k^{-1}\|_2 \|x_* - x_k\|_2^2$$

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

Result (ii) follows since once iterate becomes sufficiently close to  $x_*$ , (iii) implies that next is even closer.



# 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

## MODIFIED NEWTON METHODS

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

$$(H_k + M_k)p_k = -g_k$$

where

- $M_k$  chosen so that  $H_k + M_k$  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

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

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

# QUASI-NEWTON METHODS

Various attempts to approximate  $H_k$ :

- Finite-difference approximations:

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

for some “small” scalar  $h > 0$

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

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

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

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

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

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

## MINIMIZING A CONVEX QUADRATIC MODEL

For convex models ( $B_k$  positive definite)

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

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

$$(\text{approximately}) \min_{p \in \mathbb{R}^n} q(p) = p^T g + \frac{1}{2} p^T B p$$

## MINIMIZATION OVER A SUBSPACE

$$\odot \ D^i = (d^0 : \dots : d^{i-1})$$

$$\odot \ \text{Subspace } \mathcal{D}^i = \{p \mid p = D^i p_d \text{ for some } p_d \in \mathbb{R}^i\}$$

$$\odot \ p^i = \arg \min_{p \in \mathcal{D}^i} q(p)$$

$$\implies D^{iT} g^i = 0, \text{ where } g^i = Bp^i + g$$

$$\odot \ p^{i-1} \in \mathcal{D}^i$$

$$\implies p^i = p^{i-1} + D^i p_d^i, \text{ where}$$

$$p_d^i = \arg \min_{p_d \in \mathbb{R}^i} p_d^T D^{iT} g^{i-1} + \tfrac{1}{2} p_d^T D^{iT} B D^i p_d$$

$$= -(D^{iT} B D^i)^{-1} D^{iT} g^{i-1} = -d^{i-1T} g^{i-1} (D^{iT} B D^i)^{-1} e_i$$

$$\implies p^i = p^{i-1} - d^{i-1T} g^{i-1} D^i (D^{iT} B D^i)^{-1} e_i$$

## MINIMIZATION OVER A CONJUGATE SUBSPACE

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

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

- **B-conjugacy**:  $d_i^T B d_j = 0$  ( $i \neq j$ )

$$\implies p^i = p^{i-1} + \alpha^{i-1} d^{i-1}, \text{ where}$$

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

### Building a B-conjugate subspace

Since  $g^i$  is independent of  $\mathcal{D}^i$ , let  $d^i = -g^i + \sum_{j=0}^{i-1} \beta^{ij} d^j$

- choose  $\beta^{ij}$  so that  $d^i$  is  $B$ -conjugate to  $\mathcal{D}^i$

$$\implies \beta^{ij} = 0 \text{ } (j < i - 1), \beta^{ii-1} \equiv \beta^i = \frac{\|g_i\|_2^2}{\|g_{i-1}\|_2^2}$$

## CONJUGATE-GRADIENT METHOD

Given  $p^0 = 0$ , set  $g^0 = g$ ,  $d^0 = -g$  and  $i = 0$ .

Until  $g^i$  “small” iterate

$$\alpha^i = -g^{iT} d^i / d^{iT} B d^i$$

$$p^{i+1} = p^i + \alpha^i d^i$$

$$g^{i+1} = g^i + \alpha^i B d^i$$

$$\beta^i = \|g^{i+1}\|_2^2 / \|g^i\|_2^2$$

$$d^{i+1} = -g^{i+1} + \beta^i d^i$$

and increase  $i$  by 1

Important features

- ◉  $d^{jT} g^{i+1} = 0$  for all  $j = 0, \dots, i \implies \alpha^i = \|g^i\|_2^2 / d^{iT} B d^i$
- ◉  $g^{jT} g^{i+1} = 0$  for all  $j = 0, \dots, i$
- ◉  $g^T p^i < 0$  for  $i = 1, \dots, n \implies$  descent direction for any  $p_k = p^i$

## CONJUGATE GRADIENT METHOD GIVES DESCENT

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

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

$$p^i = p^{i-1} - \frac{g^{i-1T} d^{i-1}}{d^{i-1T} B d^{i-1}} d^{i-1} = p^{i-1} - \frac{g^T d^{i-1}}{d^{i-1T} B d^{i-1}} d^{i-1}.$$

$\implies$

$$g^T p^i = g^T p^{i-1} - \frac{(g^T d^{i-1})^2}{d^{i-1T} B d^{i-1}},$$

$\implies g^T p^i < g^T p^{i-1} \implies$  (induction)

$$g^T p^i < 0$$

since

$$g^T p^1 = -\frac{\|g\|_2^4}{g^T B g} < 0.$$

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