## Part 2: Linesearch methods for unconstrained optimization

Nick Gould (RAL)

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

MSc course on nonlinear optimization

## UNCONSTRAINED MINIMIZATION

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

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

 $\odot$  assume that  $f \in C^1$  (sometimes  $C^2$ ) and Lipschitz

often in practice this assumption violated, but not necessary

#### ITERATIVE METHODS

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

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

- 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

- $\circ$  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

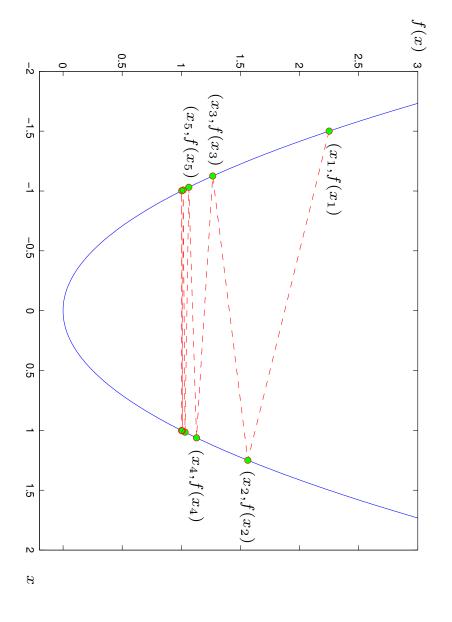
• calculate a suitable **steplength**  $\alpha_k > 0$  so that

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

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

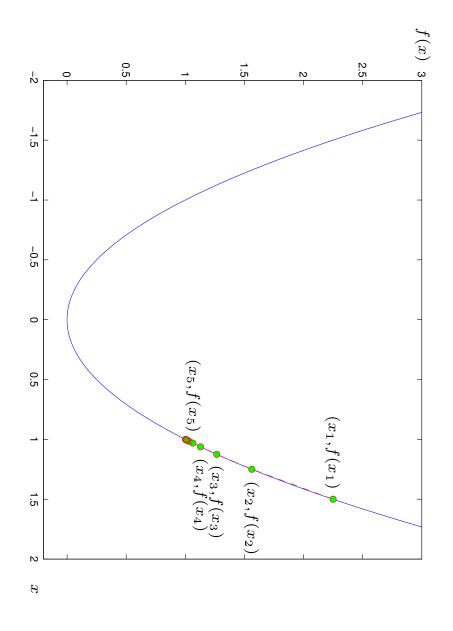
$$x_{k+1} = x_k + \alpha_k p_k$$

#### STEPS MIGHT BE TOO LONG



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

### STEPS MIGHT BE TOO SHORT



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

## PRACTICAL LINESEARCH METHODS

 $\circ$  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  $\alpha_k = \alpha^{(l)}$ 

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

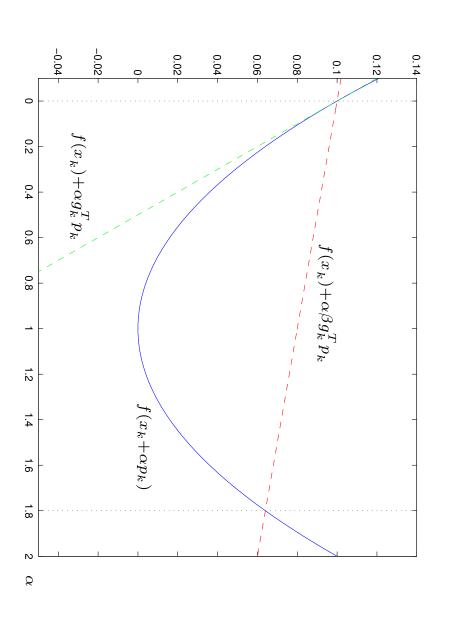
$$f(x_k + \alpha^{(l)}p_k) "<" f_k$$

#### 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.,  $\alpha_{\text{init}} = 1$ )
$$\det \alpha^{(0)} = \alpha_{\text{init}} \text{ and } l = 0$$

$$\operatorname{Until} f(x_k + \alpha^{(l)} p_k) \leq f(x_k) + \alpha^{(l)} \beta g_k^T p_k$$

$$\operatorname{set} \alpha^{(l+1)} = \tau \alpha^{(l)}, \text{ where } \tau \in (0, 1) \text{ (e.g., } \tau = \frac{1}{2})$$

$$\operatorname{and increase } l \text{ by } 1$$

$$\operatorname{Set} \alpha_k = \alpha^{(l)}$$

## SATISFYING THE ARMIJO CONDITION

a descent direction at x. Then the Armijo condition tinuous with Lipschitz constant  $\gamma(x)$ , that  $\beta \in (0,1)$  and that p is **Theorem 2.1.** Suppose that  $f \in C^1$ , that g(x) is Lipschitz con-

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

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) +

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

$$\Rightarrow f(x + \alpha p) \leq f(x) + \alpha g(x)^T p + \frac{1}{2} \gamma(x) \alpha^2 ||p||^2 
\leq f(x) + \alpha g(x)^T p + \alpha (\beta - 1) g(x)^T p 
= f(x) + \alpha \beta g(x)^T p$$

# THE ARMIJO LINESEARCH TERMINATES

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

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

#### PROOF OF COROLLARY 2.2

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

- 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

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

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

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

either

$$g_l = 0$$
 for some  $l \ge 0$ 

 $\Omega$ 

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

0r

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

#### 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

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

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

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

Let

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

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

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

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

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

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

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

$$\alpha_k \ge \alpha_{\mathrm{init}}$$

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

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.

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

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

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

# GLOBAL CONVERGENCE FOR STEEPEST DESCENT

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

either

$$g_l = 0$$
 for some  $l \ge 0$ 

Or

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

0r

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

#### 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

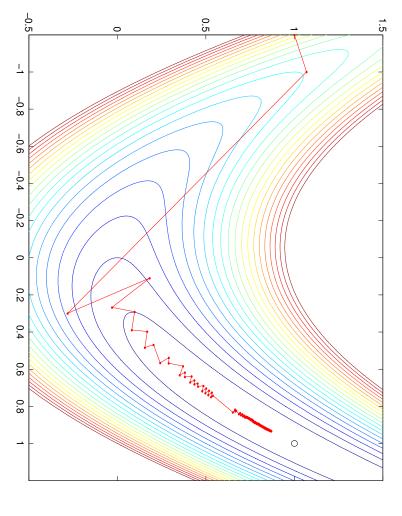
$$\lim_{k \to \infty} \min \left( |p_k^T g_k|, |p_k^T g_k| / ||p_k||_2 \right) = 0$$

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

# METHOD OF STEEPEST DESCENT (cont.)

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

### STEEPEST DESCENT EXAMPLE



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

## MORE GENERAL DESCENT METHODS

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

$$B_k p_k = -g_k$$

Then

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

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

$$p \in \mathbb{R}^n$$

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

# MORE GENERAL GLOBAL CONVERGENCE

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

either

$$g_l = 0$$
 for some  $l \ge 0$ 

0

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

0

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

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

#### PROOF OF THEOREM 2.5

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

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

and thus that

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

for any nonzero vector s. Thus

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

In addition

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

 $\downarrow \downarrow$ 

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

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

Thus

$$\frac{|\mathcal{P}_k g_k|}{||p_k||_2} \ge \frac{\lambda_{\min}}{\lambda_{\max}} ||g_k||_2$$

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

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

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

# MORE GENERAL DESCENT METHODS (cont.)

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

# CONVERGENCE OF NEWTON'S METHOD

definite. Then 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 Generic Linesearch Method with  $\alpha_{\text{init}} = 1$  and  $\beta < \frac{1}{2}$ , in which the continuous on  $\mathbb{R}^n$ . Then suppose that the iterates generated by the **Theorem 2.6.** Suppose that  $f \in \mathbb{C}^2$  and that H is Lipschitz

- (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  $\kappa \geq 0$ .  $\lim_{k \to \infty} \frac{\|x_{k+1} - x_*\|_2}{\|x_k - x_*\|_2^2}$

#### 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  $\Longrightarrow \exists k_0 \geq 0$ :

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

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

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

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

converges to zero for such k.

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

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

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

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

$$= \frac{1}{2} (p_k^T g_k + p_k^T H_k p_k) + \frac{1}{2} (p_k^T (H(z_k) - H_k) p_k)$$

$$\leq \frac{1}{2} \gamma ||z_k - x_k||_2 ||p_k||_2^2 \leq \frac{1}{2} \gamma ||p_k||_2^3$$

$$(4)$$

Now pick k sufficiently large so that

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

$$\begin{array}{l} + (3) + (4) \Longrightarrow \\ f(x_k + p_k) - f_k \leq \frac{1}{2} p_k^T g_k + \frac{1}{2} \lambda_{\min} (H_*) (1 - 2\beta) \|p_k\|_2^2 \\ \leq \frac{1}{2} (1 - (1 - 2\beta)) p_k^T g_k = \beta p_k^T g_k \end{array}$$

⇒ unit stepsize satisfies the Armijo condition for all sufficiently large

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

$$x_{k+1} - x_* = x_k - x_* - H_k^{-1} g_k = x_k - x_* - H_k^{-1} (g_k - g(x_*))$$
  
=  $H_k^{-1} (g(x_*) - g_k - H_k(x_* - x_k)).$ 

But Theorem  $1.3 \Longrightarrow$ 

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

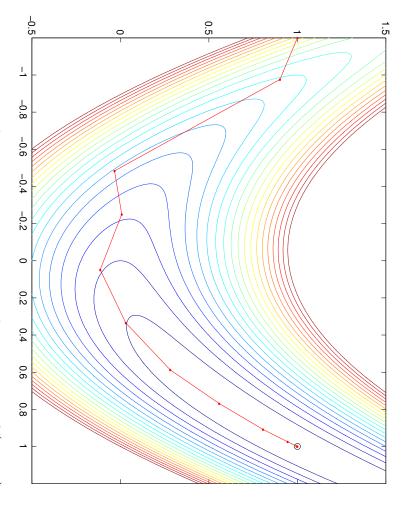
 $\downarrow \downarrow$ 

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

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

(i) and (iii) are true for all k sufficiently large 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

### NEWTON METHOD EXAMPLE



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

### 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

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

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

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

#### QUASI-NEWTON METHODS

Various attempts to approximate  $H_k$ :

• Finite-difference approximations:

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

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  $y_k^T s_k > 0$ ):

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

# MINIMIZING A CONVEX QUADRATIC MODEL

For convex models  $(B_k \text{ positive definite})$ 

$$p_k = \text{(approximate) arg min } f_k + p^T g_k^T + \frac{1}{2} p^T B_k p$$

Generic convex quadratic problem: (B positive definite)

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

## MINIMIZATION OVER A SUBSPACE

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

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

$$op^i = rg \min_{p \in \mathcal{D}^i} q(p)$$

$$\implies D^{i T} g^i = 0$$
, where  $g^i = B p^i + g$ 

$$op^{i-1} \in \mathcal{D}^i$$

$$\implies p^i = p^{i-1} + D^i p^i_d$$
, where  $p^i_d = \arg\min_{x \in \mathbb{R}^i} p^T_d D^{i T} g^{i-1}$  -

$$\begin{aligned} p_d^i &= \arg\min_{p_d \in \mathbb{R}^i} p_d^T D^{i\,T} g^{i-1} + \frac{1}{2} p_d^T D^{i\,T} B D^i p_d \\ &= - (D^{i\,T} B D^i)^{-1} D^{i\,T} g^{i-1} = - d^{i-1\,T} g^{i-1} (D^{i\,T} B D^i)^{-1} e_i \\ &\Longrightarrow p^i = p^{i-1} - d^{i-1\,T} g^{i-1} D^i (D^{i\,T} B D^i)^{-1} e_i \end{aligned}$$

# MINIMIZATION OVER A CONJUGATE SUBSPACE

Minimizer over  $\mathcal{D}^i$ :  $p^i=p^{i-1}-d^{i-1}Tg^{i-1}D^i(D^iTBD^i)^{-1}e_i$ 

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

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

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

$$\alpha^{i-1} = -\frac{d^{i-1}Tg^{i-1}}{d^{i-1}TBd^{i-1}}$$

#### Building a B-conjugate subspace

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

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

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

## CONJUGATE-GRADIENT METHOD

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

#### Important features

$$oldsymbol{0} oldsymbol{0} oldsymbol{0} oldsymbol{0} d^{j\,T}g^{i+1} = 0 \text{ for all } j = 0, \dots, i \implies \alpha^i = \|g^i\|_2^2/d^{i\,T}Bd^i$$

$$g^{j} g^{i+1} = 0 \text{ for all } j = 0, \dots, i$$

$$g^T p^i < 0 \text{ for } i = 1, \dots, n \Longrightarrow \text{ descent direction for any } p_k = p^i$$

# CONJUGATE GRADIENT METHOD GIVES DESCENT

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

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

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

 $\downarrow$ 

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

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

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

since

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

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