

# Lecture 4: Unconstrained optimization algorithms

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# Method of choice

Consider the unconstrained optimization problem to

$$\underset{\mathbf{x} \in \mathbb{R}^n}{\text{minimize}} f(\mathbf{x}), \quad (1)$$

where  $f \in C^0$  on  $\mathbb{R}^n$  ( $f$  is continuous). Mostly, we assume that  $f \in C^1$  holds ( $f$  is continuously differentiable), sometimes even  $C^2$

- Size of the problem ( $n$ )?
- Are  $\nabla f(\mathbf{x})$  and/or  $\nabla^2 f(\mathbf{x})$  available; to what cost?
- What is the goal? (Global/local minimum, stationary point?)
- What are the convexity properties of  $f$ ?
- Do we have a good estimate of the location of a stationary point  $\mathbf{x}^*$ ? (Can we use locally-only convergent methods?)

# Example: curve fitting by least-squares

- Suppose we have  $m$  data points  $(t_i, b_i)$  believed to be related as

$$x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i) = b_i, \quad i = 1, \dots, m,$$

with unknown parameters  $x_1, \dots, x_5$ . (Here,  $\exp(x) = e^x$ .)

The best description minimizes the total “residual error,” given by the norm of the residual

$$f_i(\mathbf{x}) := b_i - [x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i)], \quad i = 1, \dots, m$$

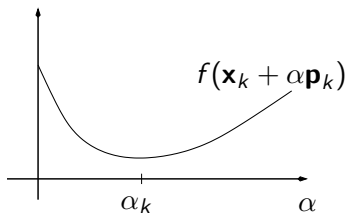
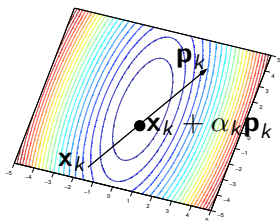
- Resulting optimization problem:

$$\min_{\mathbf{x} \in \mathbb{R}^5} f(\mathbf{x}) := \sum_{i=1}^m |f_i(\mathbf{x})|^2 = \sum_{i=1}^m (b_i - [x_1 + x_2 \exp(x_3 t_i) + x_4 \exp(x_5 t_i)])^2$$

- Very often solved problem type within numerical analysis and mathematical statistics

# Typical algorithm

- Step 0. *Starting point*:  $\mathbf{x}_0 \in \mathbb{R}^n$ . Set  $k := 0$
- Step 1. *Search direction*:  $\mathbf{p}_k \in \mathbb{R}^n$
- Step 2. *Step length*:  $\alpha_k > 0$  such that  $f(\mathbf{x}_k + \alpha_k \mathbf{p}_k) < f(\mathbf{x}_k)$  holds
- Step 3. Let  $\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k$
- Step 4. *Termination criterion*: If fulfilled, then stop!  
Otherwise, let  $k := k + 1$  and go to step 1



# Notes

- The figure was plotted using **several thousands** of function evaluations
- **Never** possible in reality! (And total waste of time)
- An “**orienteeing map**” never exists
- Most algorithms are inherently **local**, only based on info at the current point  $\mathbf{x}_k$ , that is,  $f(\mathbf{x}_k)$ ,  $\nabla f(\mathbf{x}_k)$ , and  $\nabla^2 f(\mathbf{x}_k)$
- Possibly also on previous points passed
- An algorithm is a “**near-sighted mountain climber**” when trying to reach the summit (for a max problem!)
- The mountain climber is in a deep fog and can only check her barometer for the height and feel the steepness of the slope under her feet

# Step 1: Search directions

- If  $\nabla f(\mathbf{x}_k) \neq \mathbf{0}^n$ , then  $\mathbf{p} = -\nabla f(\mathbf{x}_k)$  is a descent direction for  $f$  at  $\mathbf{x}_k$  (Part of necessary condition proof!)
- This *steepest descent direction* solves the problem to

$$\underset{\mathbf{p} \in \mathbb{R}^n: \|\mathbf{p}\|=1}{\text{minimize}} \quad \nabla f(\mathbf{x}_k)^T \mathbf{p}$$

- Suppose  $\mathbf{Q} \in \mathbb{R}^{n \times n}$  is a symmetric, positive definite matrix. Then  $\mathbf{p} = -\mathbf{Q}\nabla f(\mathbf{x}_k)$  is a descent direction for  $f$  at  $\mathbf{x}_k$ , because

$$\nabla f(\mathbf{x}_k)^T \mathbf{p} = -\nabla f(\mathbf{x}_k)^T \mathbf{Q} \nabla f(\mathbf{x}_k) < 0,$$

due to the positive definiteness of  $\mathbf{Q}$

- Special case:  $\mathbf{Q} = \mathbf{I}^n$  yields steepest descent
- Special case:  $\mathbf{Q}^{-1} = \nabla^2 f(\mathbf{x}_k)$ , if the Hessian is positive definite. This is *Newton's method*

## \*Additional requirements

- Practical criteria:

$$|\nabla f(\mathbf{x}_k)^T \mathbf{p}_k| \geq s_1 \|\nabla f(\mathbf{x}_k)\|^2, \quad \text{and} \quad \|\mathbf{p}_k\| \leq s_2 \|\nabla f(\mathbf{x}_k)\|,$$

or

$$-\frac{\nabla f(\mathbf{x}_k)^T \mathbf{p}_k}{\|\nabla f(\mathbf{x}_k)\| \cdot \|\mathbf{p}_k\|} \geq s_1, \quad \text{and} \quad \|\mathbf{p}_k\| \geq s_2 \|\nabla f(\mathbf{x}_k)\|$$

- **Purpose:** prevent the descent directions to deteriorate in quality, and prevent premature convergence
- **Interpretations:**  $\nabla f(\mathbf{x}_k)^T \mathbf{p}_k$  is the directional derivative of  $f$  at  $\mathbf{x}_k$  in the direction of  $\mathbf{p}_k$ . Make sure it stays away from zero!
- Also, make sure that  $\mathbf{p}_k$  stays bounded and that it tends to zero if and only if  $\nabla f(\mathbf{x}_k)$  does
- These conditions hold for the above examples

# Newton's method

- Steepest descent is most often *not* a very good algorithm. Why?
- It fails to take into account more than information about  $\nabla f$
- A second-order Taylor expansion:

$$f(\mathbf{x} + \mathbf{p}) - f(\mathbf{x}) \approx \varphi_{\mathbf{x}}(\mathbf{p}) := \nabla f(\mathbf{x})^T \mathbf{p} + \frac{1}{2} \mathbf{p}^T \nabla^2 f(\mathbf{x}) \mathbf{p}$$

Minimize it over  $\mathbf{p}$  by setting the gradient of  $\varphi_{\mathbf{x}}(\mathbf{p})$  to zero:

$$\nabla_{\mathbf{p}} \varphi_{\mathbf{x}}(\mathbf{p}) = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x}) \mathbf{p} = \mathbf{0}^n$$

- $n = 1$ :  $f'(x) + f''(x)p = 0 \implies p = -f'(x)/f''(x)$
- Provides descent if  $f''(x) > 0$ :  $f'(x)p = -[f'(x)]^2/f''(x) < 0$
- Corresponding story in  $\mathbb{R}^n$ :  $\mathbf{p} = -[\nabla^2 f(\mathbf{x})]^{-1} \nabla f(\mathbf{x})$ , yields descent at non-stationary points if  $\nabla^2 f(\mathbf{x})$  is positive definite!



# Why do we not always choose Newton directions? I

- **Lack of positive definiteness.**  $\nabla^2 f(\mathbf{x})$  is not positive definite (PD) (that is, some eigenvalue(s) is/are negative)
- **Solution:** add diagonal matrix so that the result is PD: if  $\lambda$  is an eigenvalue of  $\nabla^2 f(\mathbf{x})$  then for any  $\gamma \in \mathbb{R}$ ,  $\lambda + \gamma$  is an eigenvalue of  $\nabla^2 f(\mathbf{x}) + \gamma \mathbf{I}^n$ ; choose  $\gamma$  large enough to make  $\lambda + \gamma > 0$  for all eigenvalues  $\lambda$
- Note: If the value of  $\gamma$  is very large  $\implies \approx$  steepest descent
- Name: *Levenberg–Marquardt*

# Why do we not always choose Newton directions? II

- **Lack of enough differentiability.** If  $f \notin C^2$ , what do we do?
- $n = 1$ : the *secant method*:

$$f''(x_k) \approx \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}$$

- $n > 1$ : *quasi-Newton*: choose approximate matrix  $\mathbf{B}_k$  so that

$$\mathbf{B}_k(\mathbf{x}_k - \mathbf{x}_{k-1}) = \nabla f(\mathbf{x}_k) - \nabla f(\mathbf{x}_{k-1}),$$

and more choices (the above does not specify the entire matrix!)

# Why do we not always choose Newton directions? III

- **Computational burden.** It may be too much to ask for to solve a linear system many times when  $n > 1000$  or so; it is enough to do *some* work on the linear system and still get a descent property. (See book for an example)
  
- Specific choices of matrices  $\mathbf{B}_k$  lead to *quasi-Newton* methods

## Step 2: Line search

- Approximately solve the one-dimensional problem to

$$\underset{\alpha \geq 0}{\text{minimize}} \varphi(\alpha) := f(\mathbf{x}_k + \alpha \mathbf{p}_k)$$

Its optimality conditions are that

$$\varphi'(\alpha^*) \geq 0, \quad \alpha^* \cdot \varphi'(\alpha^*) = 0, \quad \alpha^* \geq 0,$$

that is,

$$\nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^T \mathbf{p}_k \geq 0, \quad \alpha^* \cdot \nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^T \mathbf{p}_k = 0, \quad \alpha^* \geq 0,$$

holds

- If  $\alpha^* > 0$ , then  $\varphi'(\alpha^*) = 0$  holds  $\implies \nabla f(\mathbf{x}_k + \alpha^* \mathbf{p}_k)^T \mathbf{p}_k = 0$
- The search direction  $\mathbf{p}_k$  is orthogonal to the gradient of  $f$  at the point  $\mathbf{x}_k + \alpha^* \mathbf{p}_k$

# Step 2: An illustration

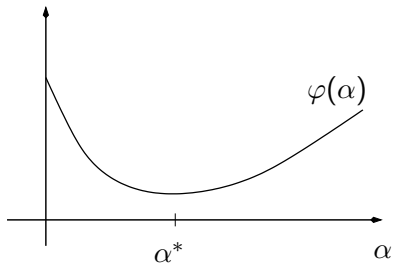
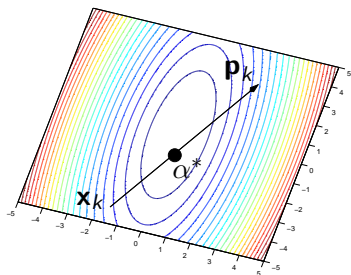


Figure: A line search in a descent direction

# Approximate line search

- No point solving the one-dimensional problem exactly! Why? The optimum to the entire problem lies elsewhere!
- *Interpolation*: Use  $f(\mathbf{x}_k), \nabla f(\mathbf{x}_k), \nabla f(\mathbf{x}_k)^T \mathbf{p}_k$  to model a quadratic function approximating  $f$  along  $\mathbf{p}_k$ . Minimize it by using the analytic formula for quadratics
- *Newton's method*: Repeat the improvements gained from a quadratic approximation:  $\alpha := \alpha - \varphi'(\alpha)/\varphi''(\alpha)$
- *Golden section*: Derivative-free method that shrinks an interval wherein a solution to  $\varphi'(\alpha) = 0$  lies

# Armijo rule, I

- **Idea:** quickly generate a step  $\alpha$  which provides “sufficient” decrease in  $f$ . Note:  $f(\mathbf{x}_k + \alpha \mathbf{p}_k) \approx f(\mathbf{x}_k) + \alpha \cdot \nabla f(\mathbf{x}_k)^\top \mathbf{p}_k$ , valid for small values of  $\alpha > 0$
- **Requirement:** we get a decrease in  $f$  which is at least a *fraction* of that predicted in the right-hand side above. Let  $\mu \in (0, 1)$  be this fraction. Acceptable step lengths are  $\alpha > 0$  satisfying

$$\varphi(\alpha) - \varphi(0) \leq \mu \alpha \varphi'(0), \quad (2a)$$

that is,

$$f(\mathbf{x}_k + \alpha \mathbf{p}_k) - f(\mathbf{x}_k) \leq \mu \alpha \nabla f(\mathbf{x}_k)^\top \mathbf{p}_k \quad (2b)$$

# Armijo rule, II

- Can add condition making  $\alpha$  also large enough (*Wolfe*)

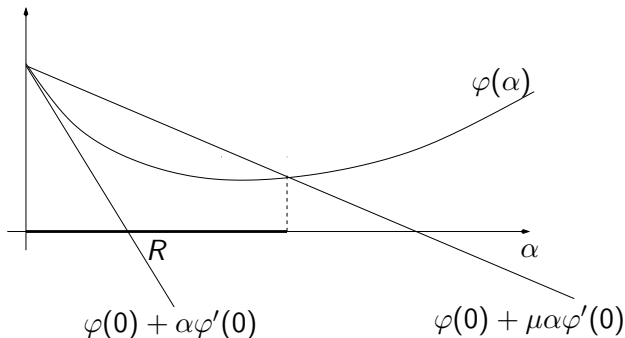


Figure: The interval ( $R$ ) accepted by the Armijo step length rule



## \*Typical convergence result

- Suppose  $f \in C^1$ , and for the starting point  $\mathbf{x}_0$  the level set  $\text{lev}_f(f(\mathbf{x}_0)) = \{\mathbf{x} \in \mathbb{R}^n \mid f(\mathbf{x}) \leq f(\mathbf{x}_0)\}$  is bounded. Consider the iterative algorithm, with the following choices for each  $k$ :
  - $\mathbf{p}_k$  satisfies the *second sufficient descent condition*;
  - $\|\mathbf{p}_k\| \leq M$ , where  $M$  is some positive constant; and
  - the *Armijo step length rule* is used

Then, the sequence  $\{\mathbf{x}_k\}$  is *bounded*, the sequence  $\{f(\mathbf{x}_k)\}$  is *descending, lower bounded* and therefore *converges*, and every *limit point of  $\{\mathbf{x}_k\}$  is stationary*

- For *convex*  $f$  much stronger convergence properties:

*Optimum exists  $\iff \{\mathbf{x}_k\}$  converges to an optimal solution*

(Theorem proved for gradient projection method later)

## Step 4: Termination criteria

- Lesson 1: Cannot terminate based on the exact optimality conditions, because  $\nabla f(\mathbf{x}) = \mathbf{0}^n$  rarely happens!
- Recommended:
  - 1  $\|\nabla f(\mathbf{x}_k)\| \leq \varepsilon_1(1 + |f(\mathbf{x}_k)|)$ ,  $\varepsilon_1 > 0$  small;
  - 2  $f(\mathbf{x}_{k-1}) - f(\mathbf{x}_k) \leq \varepsilon_2(1 + |f(\mathbf{x}_k)|)$ ,  $\varepsilon_2 > 0$  small; and
  - 3  $\|\mathbf{x}_{k-1} - \mathbf{x}_k\| \leq \varepsilon_3(1 + \|\mathbf{x}_k\|)$ ,  $\varepsilon_3 > 0$  small
- Why? Need to cover cases of very steep and very flat functions
- May need to use  $\infty$ -norm:  $\|\mathbf{x}\|_\infty := \max_{1 \leq j \leq n} |x_j|$ , for large  $n$
- Problem with the scaling of the problem: If

$$\mathbf{x}_{k-1} = (1.44453, 0.00093, 0.0000079)^T,$$

$$\mathbf{x}_k = (1.44441, 0.00012, 0.0000011)^T;$$

$$\begin{aligned} \|\mathbf{x}_{k-1} - \mathbf{x}_k\|_\infty &= \|(0.00012, 0.00081, 0.0000068)^T\|_\infty \\ &= 0.00081 \end{aligned}$$

- Small absolute error but large relative error!

# Why is the $C^1$ property important? I

- Suppose  $f$  is only in  $C^0$ , not  $C^1$ . Example:

$$f(\mathbf{x}) := \underset{i \in \{1, \dots, m\}}{\text{maximum}} \{ \mathbf{c}_i^T \mathbf{x} + b_i \}, \quad \mathbf{x} \in \mathbb{R}^n$$

- This is a piece-wise linear and convex function (see next page)
- It is differentiable almost everywhere, but *not* at the optimal solution!
- Ignoring non-differentiability may lead to the convergence to a non-optimal point. In other words, methods for minimizing non-differentiable function cannot only rely on gradient values
- Convex functions always has *subgradients*, corresponding to all the possible slopes of the function
- For more on subgradients, see Chapter 6 on Lagrangian duality!

# Why is the $C^1$ property important? II

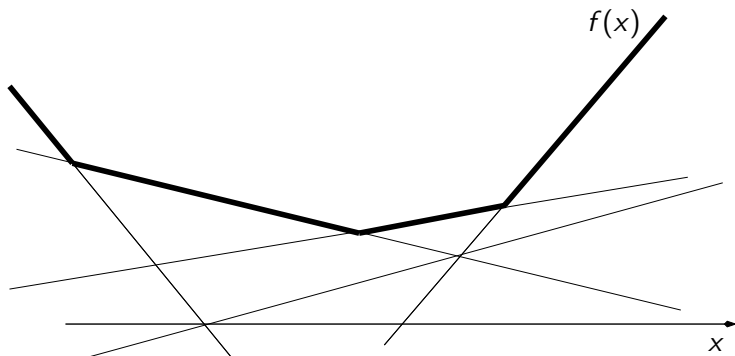
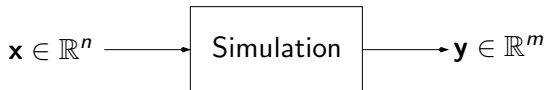


Figure: A piece-wise linear convex function

# Minimizing implicit functions, I

- Common in engineering and natural science applications that  $f$  is not explicitly given but through a **simulation**:



- Wish is to minimize a function of both  $\mathbf{x}$  and  $\mathbf{y}$ :  $f(\mathbf{x}, \mathbf{y})$ ; find the vector  $\mathbf{x}$  that gives the best *response*  $\mathbf{y}$  for  $f$
- The form of the response  $\mathbf{y} = \mathbf{y}(\mathbf{x})$  from the input  $\mathbf{x}$  is normally unknown
- Cannot differentiate  $\mathbf{x} \mapsto f(\mathbf{x}, \mathbf{y}(\mathbf{x}))$
- Two distinct possibilities!

# Minimizing implicit functions, II

- (1) *Numerical differentiation* of  $f$  by using a difference formula:
- Let  $\mathbf{e}_i = (0, 0, \dots, 0, 1, 0, \dots, 0)^T$  be the unit vector in  $\mathbb{R}^n$ . Then,

$$\begin{aligned} f(\mathbf{x} + \alpha \mathbf{e}_i) &= f(\mathbf{x}) + \alpha \mathbf{e}_i^T \nabla f(\mathbf{x}) + (\alpha^2/2) \mathbf{e}_i^T \nabla^2 f(\mathbf{x}) \mathbf{e}_i + \dots \\ &= f(\mathbf{x}) + \alpha \partial f(\mathbf{x}) / \partial x_i + (\alpha^2/2) \partial^2 f(\mathbf{x}) / \partial x_i^2 + \dots \end{aligned}$$

- So, for small  $\alpha > 0$ ,

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + \alpha \mathbf{e}_i) - f(\mathbf{x})}{\alpha} \quad (\text{forward difference})$$

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + \alpha \mathbf{e}_i) - f(\mathbf{x} - \alpha \mathbf{e}_i)}{2\alpha} \quad (\text{central difference})$$

# Minimizing implicit functions, III

- Value of  $\alpha$  typically set to a function of the machine precision; too large  $\rightarrow$  bad approximation of the partial derivative; too small  $\rightarrow$  numerical cancellation
- May work well *if* the simulation is *accurate*, otherwise bad derivative information. Requires *cheap* simulations!
- (2) *Derivative-free methods* are available. (Not counting subgradient methods, because they demand  $f$  to be convex!) Either builds explicit *models*  $\hat{f}$  of the objective function from evaluations of  $f$  at test points, or evaluates  $f$  at grid points that are moved around, shrunk or expanded. *Names and terms: Nelder–Mead, Pattern search, surrogate models, radial basis functions, ...*
- Check hand-out!

# Methods based on interpolating/approximating $f$

- Alternative: create explicit algebraic (e.g., polynomial) model  $\tilde{f}$  based on visited points  $\mathbf{x}_k$ ; solve this problem with gradient methods; evaluate its optimum in the real problem (i.e., perform a simulation); update  $\tilde{f}$  with the new information  $\implies$  minimizes the number of simulations!
- Recent application: diesel engine optimization for Volvo Powertrain and Volvo Car Corporation
- Optimize fuel consumption, keep soot/nitrogen emissions at an acceptable level
- Simulations hard (42 hours each) and response contains noise
- New method developed based on approximate (surrogate) models



## \*Trust region methods, I

- Trust region methods use quadratic models (as does Newton)
- Avoids line searches by bounding the length of the search direction, at the same time influencing its direction
- Let  $\psi_k(\mathbf{p}) := f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \mathbf{p} + \frac{1}{2} \mathbf{p}^T \nabla^2 f(\mathbf{x}_k) \mathbf{p}$
- The model  $\psi_k$  is *trusted* in a neighbourhood of  $\mathbf{x}_k$  :  $\|\mathbf{p}\| \leq \Delta_k$
- Very useful when  $\nabla^2 f(\mathbf{x}_k)$  is not positive semi-definite

## \*Trust region methods, II

- Relatively easy to minimize  $\psi_k(\mathbf{p})$  subject to  $\|\mathbf{p}\| \leq \Delta_k$
- Idea: when  $\nabla^2 f(\mathbf{x}_k)$  is badly conditioned,  $\Delta_k$  should be small (more of a steepest descent method); if well conditioned,  $\Delta_k$  should be large to allow for unit steps (Newton! fast convergence)
- If  $\Delta_k$  is small enough,  $f(\mathbf{x}_k + \mathbf{p}_k) < f(\mathbf{x}_k)$  holds
- Even if  $\nabla f(\mathbf{x}_k) = \mathbf{0}^n$  holds,  $f(\mathbf{x}_k + \mathbf{p}_k) < f(\mathbf{x}_k)$  still holds, if  $\nabla^2 f(\mathbf{x}_k)$  is not positive definite
- Progress from stationary points if at saddle points or local maxima

## \*Trust region methods, III

- Update of trust region size based on a measure of similarity between the model  $\psi_k$  and  $f$ : Let

$$\rho_k = \frac{f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{p}_k)}{f(\mathbf{x}_k) - \psi_k(\mathbf{p}_k)} = \frac{\text{actual reduction}}{\text{predicted reduction}}$$

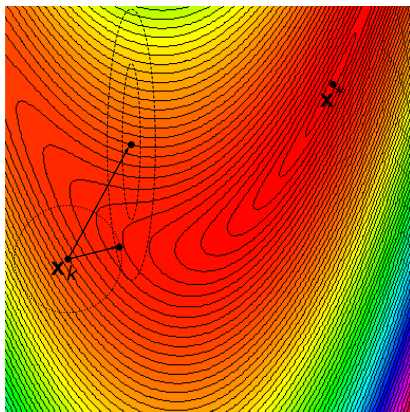
If  $\rho_k \leq \mu$  let  $\mathbf{x}_{k+1} = \mathbf{x}_k$  (unsuccessful step), else  
 $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{p}_k$  (successful step)

Value of  $\Delta_{k+1}$  depends on  $\rho_k$ :

$$\begin{aligned} \rho_k \leq \mu &\implies \Delta_{k+1} = \frac{1}{2}\Delta_k, \\ \mu < \rho_k < \eta &\implies \Delta_{k+1} = \Delta_k, \\ \rho_k \geq \eta &\implies \Delta_{k+1} = 2\Delta_k \end{aligned}$$

# \*Trust region methods, IV

Figure 4 illustrates the trust region subproblem



**Figure:** Trust region and line search step. The ellipses are level curves of the quadratic model; the circle defines the trust region

## \*Conjugate gradient methods, I

- Algorithm for strictly convex quadratic programs to minimize  $f(\mathbf{x}) := \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x} - \mathbf{q}^T\mathbf{x}$ , that is, solve  $\mathbf{Q}\mathbf{x} = \mathbf{q}$
- Non-quadratic extensions available
- Basic scheme:

$$\mathbf{p}_0 = -\nabla f(\mathbf{x}_0); \quad (3a)$$

$$\mathbf{p}_k = -\nabla f(\mathbf{x}_k) + \beta_k \mathbf{p}_{k-1}, \quad k = 1, 2, \dots, n-1, \quad (3b)$$

where

$$\beta_k = \frac{\nabla f(\mathbf{x}_k)^T \nabla f(\mathbf{x}_k)}{\nabla f(\mathbf{x}_{k-1})^T \nabla f(\mathbf{x}_{k-1})} \quad (3c)$$

- Use exact line search

## \*Conjugate gradient methods, II

Crucial properties:

- (a) Step  $k$  minimizes  $f$  over a  $k$ -dimensional manifold; after at most  $n$  steps we find the optimal solution
- (b) All directions  $\mathbf{p}_k$  are “conjugate”, that is,  $\mathbf{p}_i^T \mathbf{Q} \mathbf{p}_j = 0$  for  $i \neq j$   
(Type of orthogonality; generation a type of Gram–Schmidt procedure applied to the negative gradients)
- (c) Need only store the previous gradient to get new direction
- (d) Strictly better convergence than steepest descent
- (e) Direction vector  $\mathbf{p}_i$  is an eigenvector corresponding to a largest eigenvalue  $\lambda_i$  not yet found
- (f) Meaning: Takes care of most difficult part of the problem first. Less sensitive to the size of the condition number  $\kappa(\mathbf{Q}) := \lambda_n/\lambda_1$  than steepest descent