Lecture 2

Iterative Methods

Computational Mathematics

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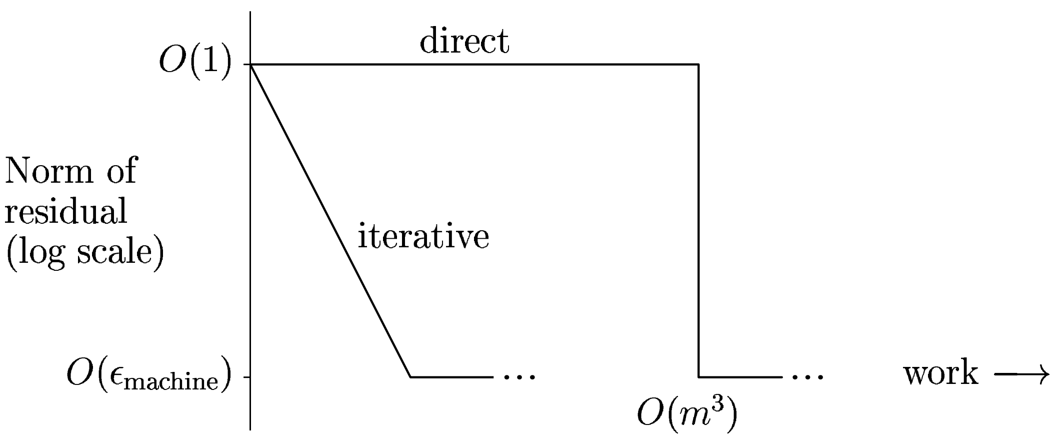
Direct vs Iterative Methods

- Direct methods: compute the exact solution after a finite number of steps (in exact arithmetic); Gaussian elimination, QR factorization, etc.
- Iterative methods: produce a sequence of approximations $x^{(0)}, x^{(1)}, \ldots$ that hopefully converge to the true solution; Jacobi, Conjugate Gradient (CG), GMRES, BiCG, etc.



Iterative Methods

- The basic idea of iterative methods is to construct a sequence of vectors $x^{(k)}$ such that

$$\mathrm{x} = \lim_{\mathrm{k}\to\infty} \mathrm{x}^{(\mathrm{k})},$$

where x is the solution to the system

$$Ax = b \tag{1}$$

- To start with, we consider iterative methods in the form

$$x^{(0)} \text{ given, } x^{(k+1)} = Bx^{(k)} + f, \quad k \geqslant 0 \tag{2}$$

- The iterative method is said to be consistent with $Ax = b$ if B and f are such that $x = Bx + f$

Convergence of Iterative Methods

- Let

$$e^{(k)} = x^{(k)} - x.$$

The condition of convergence amounts to requiring that

$$\lim_{k\to\infty} e^{(k)} = 0 \Leftrightarrow \lim_{k\to\infty} \|e^{(k)}\| = 0$$

- The choice of the norm does not influence the result since in $\mathbb{R}^{n\times n}$ all norms are equivalent

Theorem 2.1: Convergence

Let (2) be a consistent method. Them the sequence of vectores $\{x^{(k)}\}$ converges to the solution of (1) for any choice of $\{x^{(0)}\}$ if and only if $\rho(B) < 1$.

- A sufficient condition for convergence to hold is that $\|B\| < 1$
- It reasonable to expect that the convergence is faster when $\rho(B)$ is smaller

Classes of Matrices

- Symmetric Positive Definite (SPD):

$$x^T A x > 0, \qquad \text{for } x \neq 0$$

- Strictly Row Diagonal Dominant (SRDD):

$$|a_{ii}| > \sum_{j=1, j\neq i}^{n} |a_{ij}|, \qquad i = 1, \ldots, n$$

- Strictly Column Diagonal Dominant (SCDD):

$$|a_{jj}| > \sum_{i=1, i\neq j}^{n} |a_{ij}| \qquad j = 1, \ldots, n$$

Linear Iterative Methods

Consistent Linear Iterative Methods

- Let $A = P - N$, where P and N are two suitable matrices and P is nonsingular; P is called preconditioning matrix or preconditioner
- Given $x^{(0)}$ one can compute $x^{(k)}$ by solving the system

$$Px^{(k+1)} = Nx^{(k)} + b, \quad k \geqslant 0 \tag{3}$$

- The iteration matrix is $B = P^{-1}N$ and $f = P^{-1}b$
- The iterative method (3) can be written as

$$x^{(k+1)} = x^{(k)} + P^{-1}r^{(k)}, \quad k \geqslant 0,$$

where

$$r^{(k)} = b - Ax^{(k)},$$

denotes the residual vector at step k

SPD Matrices

- If $A \in \mathbb{R}^{n\times n}$ is SPD, then $(x, y)_A = x^T Ay$ defines an inner product on $\mathbb{R}^n$ and $\|x\|_A = (x^T Ax)^{1/2}$ is a norm on $\mathbb{R}^n$

Theorem 2.2: Monotone Convergence (*)

Let $A = P - N$, with A and P be SPD. If $2P - A$ is PD, the iterative method is convergent for any choice of $x^{(0)}$ and

$$\rho(B) = \|B\|_A = \|B\|_P < 1.$$

Moreover, the convergence is monotone w.r.t. $\|\cdot\|_A$ and $\|\cdot\|_P$:

$$\|e^{(k+1)}\|_A < \|e^{(k)}\|_A, \text{ and } \|e^{(k+1)}\|_P < \|e^{(k)}\|_P.$$

Theorem 2.3: Monotone Convergence (*)

If A is SPD and $P + P^T - A$ is PD, then P is invertible and the iterative method is monotonically convergent w.r.t. $\|\cdot\|_A$ and $\rho(B) = \|B\|_A < 1$.

Jacobi Method

- Let A be a matrix with nonzero diagonal entries and

$$P = D, \quad N = D - A,$$

where D is the diagonal matrix of the diagonal entries of A

- The iteration matrix of the Jacobi method is given by

$$B_J = D^{-1}(D - A) = I - D^{-1}A$$

- Jacobi method:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=1, j\neq i}^{n} a_{ij} x_j^{(k)} \right], \quad i = 1, \dots, n$$

Jacobi Over-Relaxation Method (JOR)

- The iteration matrix is given by

$$B_J(\omega) = \omega B_J + (1 - \omega) I$$

- JOR method:

$$x_i^{(k+1)} = \frac{\omega}{a_{ii}} \left[b_i - \sum_{j=1, j\neq i}^{n} a_{ij} x_j^{(k)} \right] + (1-\omega) x_i^{(k)}, \quad i = 1, \dots, n$$

- Exercise 1: JOR is consistent for any $\omega \neq 0$ and the residual form is:

$$x^{(k+1)} = x^{(k)} + \omega D^{-1} r^{(k)}, \quad k \geqslant 0$$

- For $\omega = 1$ JOR coincides with the Jacobi method

Optimal Choice of Parameter

Theorem 2.4: Optimal Choice of Parameter for JOR

Assume that B_J has real eigenvalues and $\rho(B_J) < 1$. Then $\rho(B_J(\omega))$ becomes minimal for the relaxation parameter

$$\omega_{opt} = \frac{2}{2 - \lambda_{max} - \lambda_{min}}$$

and the spectral radius

$$\rho_{opt} = \frac{\lambda_{max} - \lambda_{min}}{2 - \lambda_{max} - \lambda_{min}},$$

where λ_{min} and λ_{max} denote the smallest and the largest eigenvalue of B, respectively.

- In the case $\lambda_{max} \neq -\lambda_{min}$ the convergence of the Jacobi method with optimal relaxation parameter is faster then the convergence of the Jacobi method without relaxation

Gauss-Seidel Method

- Let A be a matrix with nonzero diagonal entries and

$$P = D - E, \quad N = F,$$

  where D is the diagonal matrix ($d_{ii} = a_{ii}$), E is the lower triangular matrix ($e_{ij} = -a_{ij}$, $i > j$) and F is the upper triangular matrix ($f_{ij} = -a_{ij}$, $j > i$)
- The iteration matrix of the Gauss-Seidel method is given by

$$B_{GS} = (D - E)^{-1} F$$

- Gauss-Seidel:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right], \quad i = 1, \ldots, n$$

Gauss-Seidel Over-Relaxation Method (SOR)

- SOR:

$$x_i^{(k+1)} = \frac{\omega}{a_{ii}} \left[b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)} \right] + (1-\omega) x_i^{(k)}, \; i = 1, \dots, n$$

- The method can be written as

$$(I - \omega D^{-1} E) x^{(k+1)} = [(1-\omega) I + \omega D^{-1} F] x^{(k)} + \omega D^{-1} b,$$

and the iteration matrix is

$$B_{GS}(\omega) = (I - \omega D^{-1} E)^{-1} [(1-\omega) I + \omega D^{-1} F]$$

- Exercise 2: The SOR method is consistent for any $\omega \neq 0$ and for $\omega = 1$ and the residual form is:

$$x^{(k+1)} = x^{(k)} + \left(\frac{1}{\omega} D - E \right)^{-1} r^{(k)}, \quad k \geqslant 0$$

- For $\omega = 1$ it coincides with the Gauss-Seidel method

Convergence of Jacobi and Gauss-Seidel Methods

Theorem 2.5: Convergence of Jacobi and Gauss-Seidel

If A is SRDD, then the Jacobi and Gauss-Seidel methods are convergent.

Theorem 2.6: Monotone Convergence of Jacobi (∗)

If A and $2P - A$ are SPD, then the Jacobi method is convergent for any choice of $x^{(0)}$ and

$$\rho(B_J) = \|B_J\|_A = \|B_J\|_D < 1.$$

Moreover, the convergence is monotone w.r.t. $\|\cdot\|_A$ and $\|\cdot\|_D$.

Theorem 2.7: Convergence of JOR for SPD Matrices

If A is SPD and $0 < \omega < 2/\rho(D^{-1}A)$, then the JOR method is convergent.

Convergence of Jacobi and Gauss-Seidel Methods

Theorem 2.8: Convercence of JOR

If the Jacobi method is convergent, then the JOR method converges if $0 < \omega \leqslant 1$.

Theorem 2.9: Monotone Convergence of Gauss-Seidel

If A is SPD then the Gauss-Seidel method is monotonically convergent with respect to the norm $\| \cdot \|_A$.

Theorem 2.10: Convergence of SOR

For any $\omega \in \mathbb{R}$ we have $\rho(B_{GS}(\omega)) \geqslant |\omega - 1|$. Therefore the SOR method fails to converge if $\omega \leqslant 0$ or $\omega \geqslant 2$.

Theorem 2.11 (Ostrowski): Monotone Convergence of SOR

If A is SPD, then the SOR method is convergent if and only if $0 < \omega < 2$. Moreover, it is monotonically convergent w.r.t. $\| \cdot \|_A$.

Richardson Method

Richardson Method

- Let
$$R = I - P^{-1}A$$
the iteration matrix associated to the method
$$x^{(k+1)} = Rx^{(k)} + P^{-1}b \Leftrightarrow x^{(k+1)} = x^{(k)} + P^{-1}r^{(k)}, \quad k \geqslant 0$$
- Stationary Richardson method:
$$x^{(k+1)} = x^{(k)} + \alpha P^{-1}r^{(k)}, \quad k \geqslant 0$$
- Nonstationary Richardson method:
$$x^{(k+1)} = x^{(k)} + \alpha_k P^{-1}r^{(k)}, \quad k \geqslant 0$$
- The iteration matrix of the $k-$th step for these methods is
$$R(\alpha_k) = I - \alpha_k P^{-1}A$$

Richardson Method

- If $P = I$, the methods is called nonpreconditioned
- The Jacobi (resp. Gauss-Seidel) method is stationary Richardson method with $\alpha = 1$ and $P = D$ (resp. $P = D - E$)
- Algorithm: Nonstationary Richardson Method

  $x^{(0)}$ and P given; $r^{(0)} = b - Ax^{(0)}$
  for $k = 0, 1, \ldots$
  solve $Pz^{(k)} = r^{(k)}$ % compute preconditioned residual
  compute α_k % acceleration parameter
  $x^{(k+1)} = x^{(k)} + \alpha_k z^{(k)}$ % update the solution
  $r^{(k+1)} = r^{(k)} - \alpha_k Az^{(k)}$ % update the residual
  until convergence

Convergence of Richardson Method

Theorem 2.12: Convergence

For any nonsingular matrix P, the stationary Richardson method is convergent if and only if

$$\frac{2\text{Re } \lambda_i}{\alpha|\lambda_i|^2} > 1 \quad \forall i = 1, \ldots, n,$$

where $\lambda_i \in \mathbb{C}$ are the eingenvalues of $P^{-1}A$.

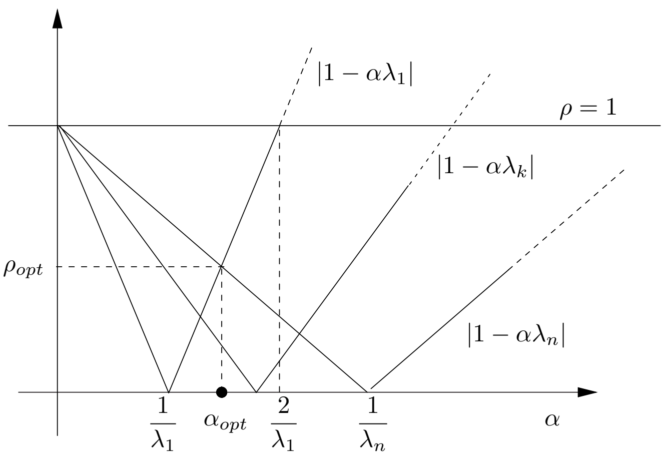
- Remark: If the sign of the real parts of the eigenvalues of $P^{-1}A$ is not constant, the stationary Richardson method cannot converge.

Convergence of Richardson Method

Theorem 2.13: Convergence

Let P be a nonsingular matrix and $P^{-1}A$ with positive real eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n > 0$. Then, the stationary Richardson method is convergent if and only if $0 < \alpha < 2/\lambda_1$. Moreover, if $\alpha = \alpha_{opt} = 2/(\lambda_1 + \lambda_n)$ then $\rho(R(\alpha))$ is minimum and

$$\rho_{opt} = \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}.$$



Convergence of Richardson Method for SPD Matrices

- If $P^{-1}A$ is SPD, the convergence of the Richardson method is monotone with respect to either $\|\cdot\|_2$ and $\|\cdot\|_A$
- In such case

$$\alpha_{opt} = \frac{2\|P^{-1}A\|_2}{K_2(P^{-1}A)+1} \quad \text{and} \quad \rho_{opt} = \frac{K_2(P^{-1}A)-1}{K_2(P^{-1}A)-1}$$

Theorem 2.14: Convergence for SPD matrices

If A is SPD, then the non preconditioned stationary Richardson method is convergent for any choice of $x^{(0)}$ and

$$\|e^{(k+1)}\|_A \leqslant \rho(R(\alpha))\|e^{(k)}\|_A, \quad k \leqslant 0.$$

The same result hold for the preconditioned Richardson method, provided that the matrices P, A and $P^{-1}A$ are SPD.

Preconditioning Matrices

- All methods can be regarded as being methods for solving

$$P^{-1}Ax = P^{-1}b$$

- This last is called *preconditioned system*, being P the preconditioning matrix or left preconditioner
- Right preconditioners can also be introduced and the system is transformed as

$$P_L^{-1}AP_R^{-1}y = P_L^{-1}b, \quad y = P_R x$$

- Optimal preconditioner: a preconditioner which is able to make the number of iterations required for convergence independent of the size of the system
- $P = A$ is optimal but inefficient; $P = I$ is efficient but not useful

Choice of Preconditioners

- In the choice of the preconditioner the computational cost and memory requirements must be taken into account
- Diagonal preconditioners: choosing P as the diagonal off A is generally effective if A is SPD. An usual choice in the non symmetric case is to set

$$p_{ii} = \left(\sum_{j=1}^{n} a_{ij}^2 \right)^{1/2}$$

- Polynomial preconditioners: the preconditioner matrix is defined as

$$P^{-1} = p(A),$$

  where p is a polynomial in A, usually of low degree
- ...

Gradient Method

Gradient Method for SPD Matrices

- The expression of the optimal parameter requires the knowledge of the extremal eigenvalues of $P^{-1}A$
- Exercise 3: For SPD matrices, solving $Ax = b$ is equivalent to finding the minimizer $x \in \mathbb{R}^n$ of the quadratic form

$$\phi(y) = \frac{1}{2}y^T Ay - y^T b \qquad \text{(energy of the system)}$$

- Goal: Determine the minimizer $x \in \mathbb{R}^n$ of ϕ. Starting from $x^{(0)} \in \mathbb{R}^n$,

$$x^{(k+1)} = x^{(k)} + \alpha_k d^{(k)}, \quad k \geqslant 0,$$

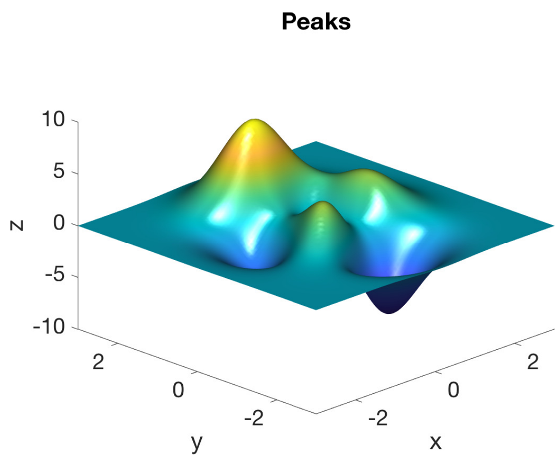
where $d^{(k)}$ is a descent direction

Example: Finding Minima

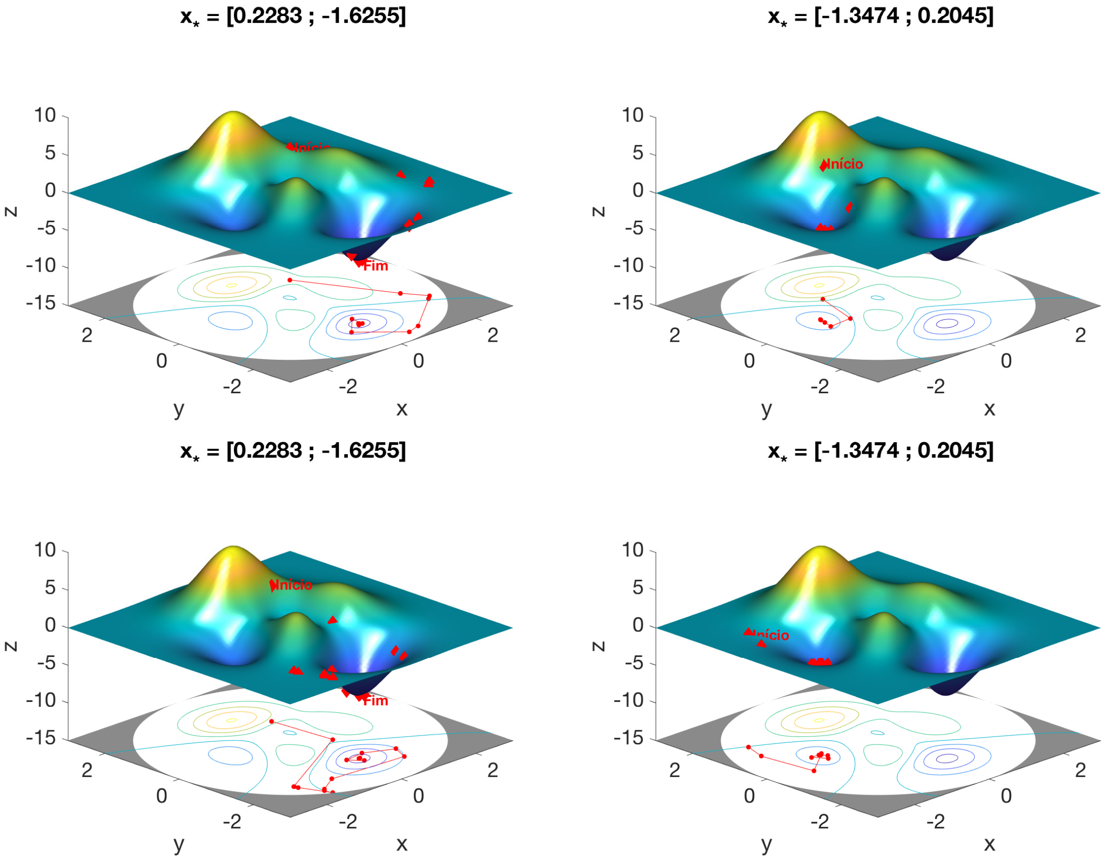
- Compute the minimizer of

$$peaks : D \subset \mathbb{R}^2 \longrightarrow \mathbb{R}$$

$$\begin{aligned} z &= peaks\,(x, y) \\ &= 3(1-x)^2 e^{-x^2-(y+1)^2} \\ &\quad -10\left(\frac{x}{5} - x^3 - y^5\right) e^{-x^2-y^2} \\ &\quad -\frac{1}{3} e^{-(x+1)^2-y^2} \end{aligned}$$

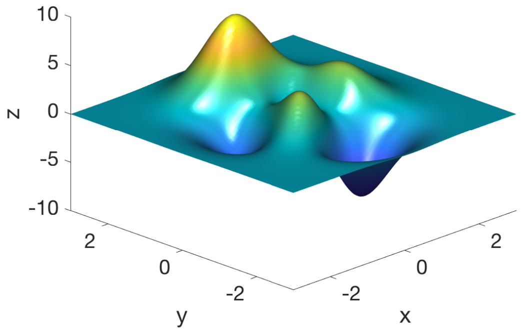


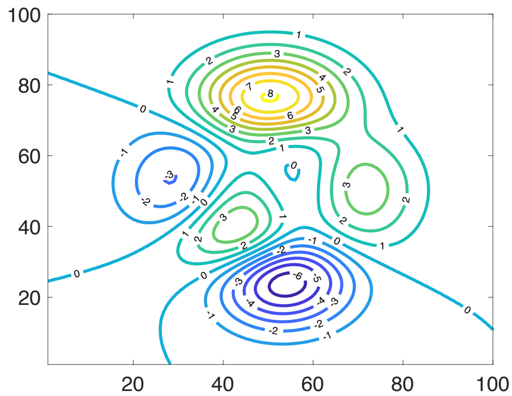
An Iterative Process



Directional Derivative and Gradient Vector

- Directional derivative: $D_d\phi(x) \;=\; \nabla\phi(x)^T d$

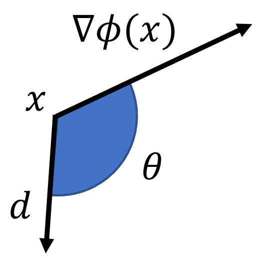




- The directional derivative is given by

$$D_d\phi(x) \;=\; \nabla\phi(x)^T d \;=\; \|\nabla\phi(x)\|\|d\|\cos\theta,$$

where θ the angle between $\nabla\phi(x)$ and the direction d

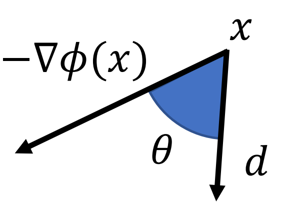


Directional Derivative and Gradient Vector

- Exercise 4: If $\phi \in C^1(\Omega)$ the maximum (resp. minimum) of the directional derivative $D_d\phi(x)$ occurs when d has the same direction as the gradient vector $\nabla\phi(x)$ (resp. $-\nabla\phi(x)$)
- Descent direction: $d \in \mathbb{R}^n$ is a descent direction of ϕ in x if exists $\bar{t} > 0$ such that $\phi(x + td) < \phi(x)$, for all $t \in (0, \bar{t})$
- Exercise 5: If the angle between d and $-\nabla\phi(x)$ is less than $\pi/2$, i.e.

$$-\nabla\phi(x)^T d \;>\; 0,$$

then d is a descent direction

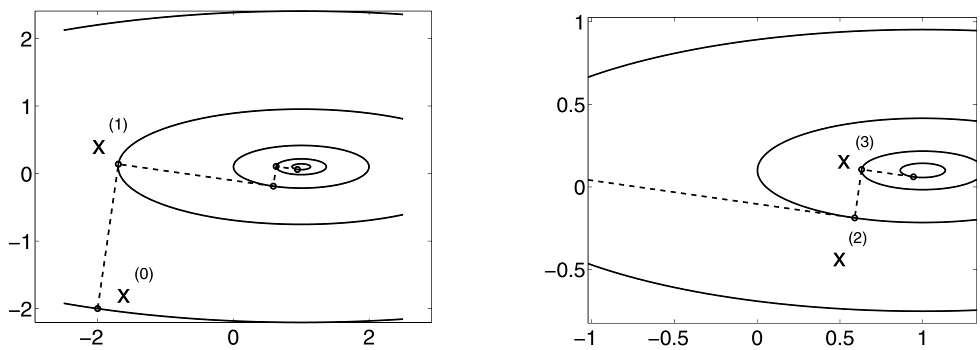


Gradient/Steepest Descent Method

- Starting from a point $x^{(0)} \in \mathbb{R}^n$, the step $k+1$ is computed as

$$x^{(k+1)} = x^{(k)} + \alpha_k d^{(k)},$$

where $d^{(k)} = -\nabla\phi(x^{(k)})$



- Exercise 6: Prove that

$$\nabla\phi(x^{(k)}) = Ax^{(k)} - b = -r^{(k)},$$

so the gradient method, as the Richardson method, moves at each step k along the direction $r^{(k)}$

Computing the Acceleration Parameter

- To compute α_k let us write $\phi(x^{(k+1)})$ as a function of a parameter α,

$$\phi(x^{(k+1)}) = \frac{1}{2}(x^{(k)} + \alpha r^{(k)})^T A(x^{(k)} + \alpha r^{(k)}) - (x^{(k)} + \alpha r^{(k)})^T b$$

- Exercise 7: Differentiating with respect to α, the value of α_k (which depends only on the residual) is

$$\alpha_k = \frac{{r^{(k)}}^T r^{(k)}}{{r^{(k)}}^T A r^{(k)}}$$

Gradient/Steepest Descent Method

- Algorithm: Gradient/Steepest Descent Method

$x^{(0)}$ given;
for $k = 0, 1, \dots$

$$r^{(k)} = b - Ax^{(k)} \quad \text{\% compute residual}$$

$$\alpha_k = \frac{{r^{(k)}}^T r^{(k)}}{{r^{(k)}}^T A r^{(k)}} \quad \text{\% acceleration parameter}$$

$$x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)} \quad \text{\% update solution}$$

until convergence

Theorem 2.15: Convergence

Let A be SPD. Then the gradient method is convergent for any choice of $x^{(0)}$ and

$$\|e^{(k+1)}\|_A \leqslant \frac{K_2(A) - 1}{K_2(A) + 1}\|e^{(k)}\|_A.$$