Lecture 1

Iterative Methods

New Directions in Mathematics

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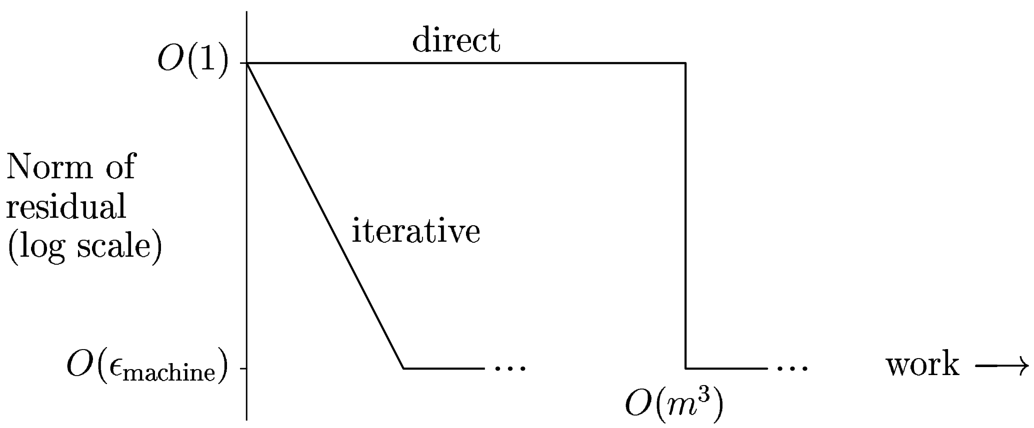
Direct vs Iterative Methods

- 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 1.1: Convergence

Let (2) be a consistent method. Then 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):

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

- Exercise 1.1: If $A \in \mathbb{R}^{n\times n}$ is SPD, then

$$(x, y)_A = x^T A y$$

defines an inner product on $\mathbb{R}^n$ and

$$\|x\|_A = (x^T A x)^{1/2}$$

is a norm on $\mathbb{R}^n$.

- Strictly Row Diagonal Dominant (SRDD):

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

Linear Iterative Methods

Consistent Linear Iterative Methods

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

$$Px^{(k+1)} = (P - A)x^{(k)} + b, \quad k \geqslant 0 \tag{3}$$

- The iteration matrix is

$$B = P^{-1}(P - A) = I - P^{-1}A$$

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: Monotone Converrgence (∗)

Theorem 1.2: Monotone Convergence (∗)

Let $A = P - (P - A)$, 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 1.3: 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

$$A = D - L - U,$$

where $D = (a_{ii})$ (diagonal), $L = (-a_{ij}), i > j$, (lower triangular and $U = (-a_{ij}), j > i$ (upper triangular) matrices

- Let

$$P = D$$

- The iteration matrix of the Jacobi method is given by

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

- Jacobi method:

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

Gauss-Seidel Method

- Let A be a matrix with nonzero diagonal entries and

$$P = D - L$$

- The iteration matrix of the Gauss-Seidel method is given by

$$B_{GS} = (D - L)^{-1} U = I - (D - L)^{-1} A$$

- Gauss-Seidel:

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

Convergence of Jacobi and Gauss-Seidel Methods

Theorem 1.4: Convergence of Jacobi and Gauss-Seidel

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

Theorem 1.5: Monotone Convergence of Jacobi $(*)$

If A and $2D - A$ 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 1.6: Monotone Convergence of Gauss-Seidel

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

Jacobi Over-Relaxation Method (JOR)

- The iteration matrix is given by

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

- JOR method:

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

- Exercise 1.2: 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 1.7: 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 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

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

and the iteration matrix is

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

- Exercise 1.3: The SOR method is consistent for any $\omega \neq 0$ and for $\omega = 1$ and the residual form is:

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

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

Convergence of Jacobi and Gauss-Seidel Methods

Theorem 1.8: Convergence of JOR for SPD Matrices

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

Theorem 1.9: Convercence of JOR

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

Theorem 1.10: 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 1.11 (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. $\|\cdot\|_A$.

HW Exercise

- Exercise 1.4: Consider the SOR method for $Ax = b$.
  1. Consider the tridiagonal matrix A with 2 on the diagonal and -1 above and below the diagonal. Construct the right-hand side vector so that $x = [1, 1, ..., 1]^T$ is the true solution.
  2. For each value of $\omega = 1, 1.01, 1.02, ..., 1.99, 2.0$, apply 100 iterations of SOR starting with $x^{(0)} = 0$. Do this for A of order 10, 20, and 50. Measure the error at the end of 100 iterations, call it e, and set $p = \sqrt[100]{e}$. The value of p is the "average" rate of convergence of the iteration; the error was reduced by this much on each iteration. Note that the error of $x^{(0)}$ is 1.
  3. For each of the three cases make a performance plot of p versus ω and estimate the optimum value of ω. If the plot is too coarse, make additional runs to fill in the gaps.
  4. Discuss the behavior of the performance profiles and their implications for the difficulty of finding optimum SOR factors.

Richardson Method

Richardson Method

- Let

$$R = I - P^{-1}A$$

the iteration matrix associated to the method

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

- 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. $P = D - L$)
- 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
      $r^{(k+1)} = r^{(k)} - \alpha_k A z^{(k)}$ % update the residual
  until convergence

Convergence of Richardson Method

Theorem 1.12: 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 eigenvalues of $P^{-1}A$.

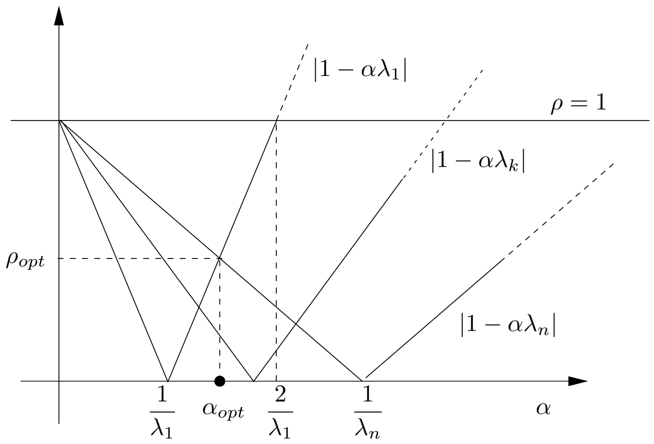
- Note: If the sign of the real parts of the eigenvalues of $P^{-1}A$ is not constant, the stationary Richardson method cannot converge

Convergence of Richardson Method

Theorem 1.13: Convergence

Let P be a nonsingular matrix and $P^{-1}A$ with positive real eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n > 0$. 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 1.14: 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 1.5: 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 $x^{(0)} \in \mathbb{R}^n$,

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

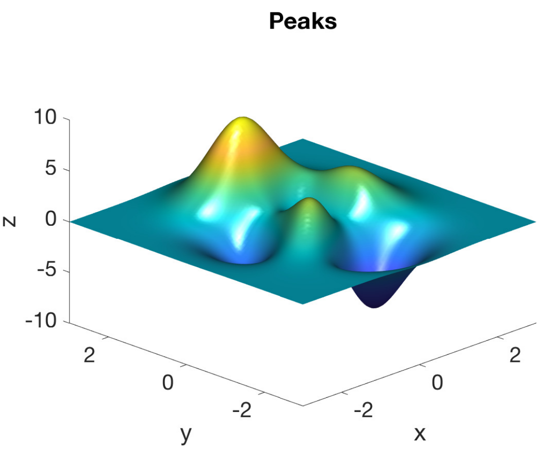
where $p^{(k)}$ is a descent direction

Example: Finding Minima

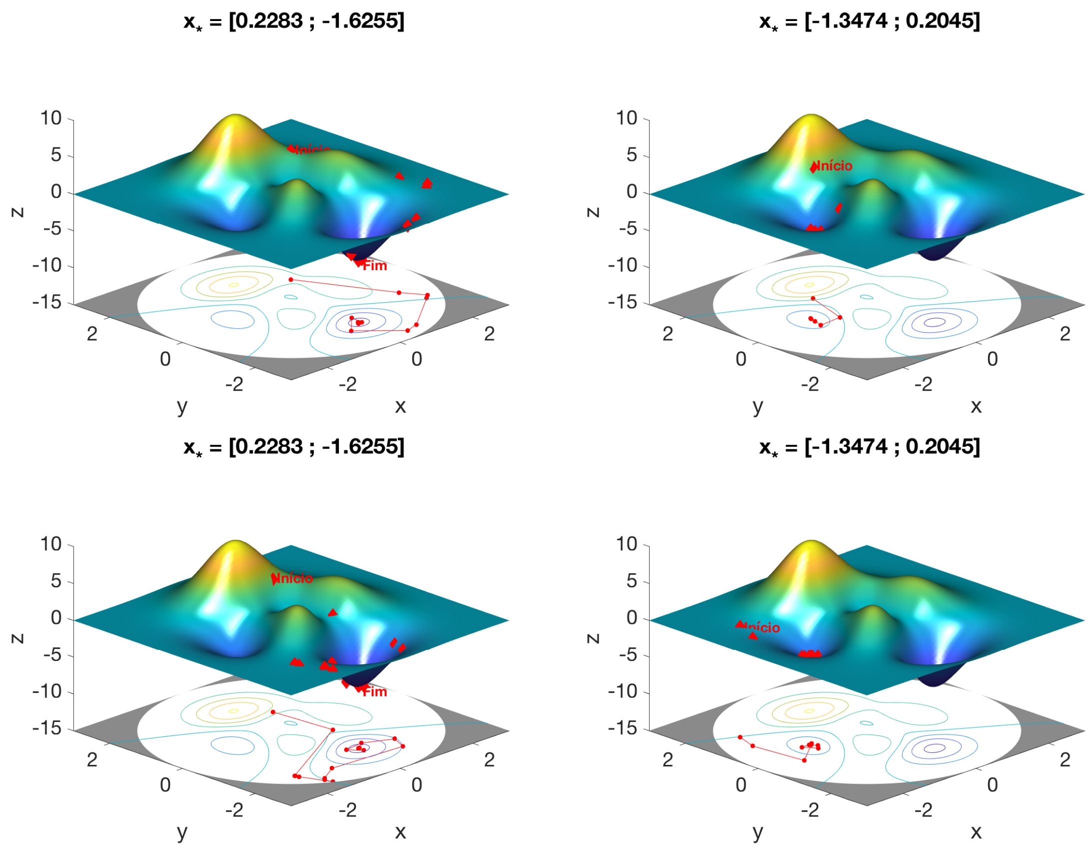
- Compute the minimizer of

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

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

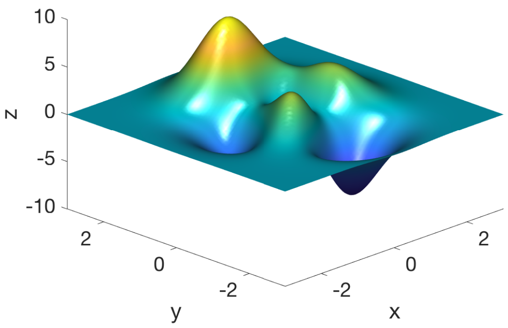


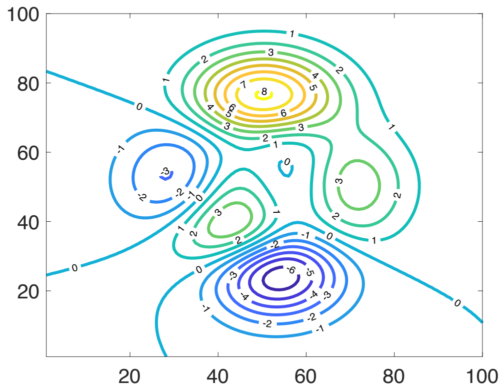
An Iterative Process



Directional Derivative and Gradient Vector

- Directional derivative: $D_p\phi(x) \;=\; \nabla\phi(x)^T p$

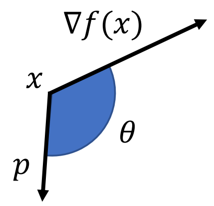




- The directional derivative is given by

$$D_p\phi(x) \;=\; \nabla\phi(x)^T p \;=\; \|\nabla\phi(x)\|\|p\|\cos\theta,$$

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

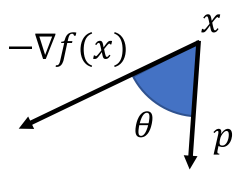


Directional Derivative and Gradient Vector

- Exercise 1.6: If $\phi \in C^1(\Omega)$ the maximum (resp. minimum) of the directional derivative $D_p\phi(x)$ occurs when p has the same direction as the gradient vector $\nabla\phi(x)$ (resp. $-\nabla\phi(x)$).
- Descent direction: $p \in \mathbb{R}^n$ is a descent direction of ϕ in x if exists $\bar{t} > 0$ such that $\phi(x + tp) < \phi(x)$, for all $t \in (0, \bar{t})$
- Exercise 1.7: If the angle between p and $-\nabla\phi(x)$ is less than $\pi/2$, i.e.

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

then p is a descent direction.

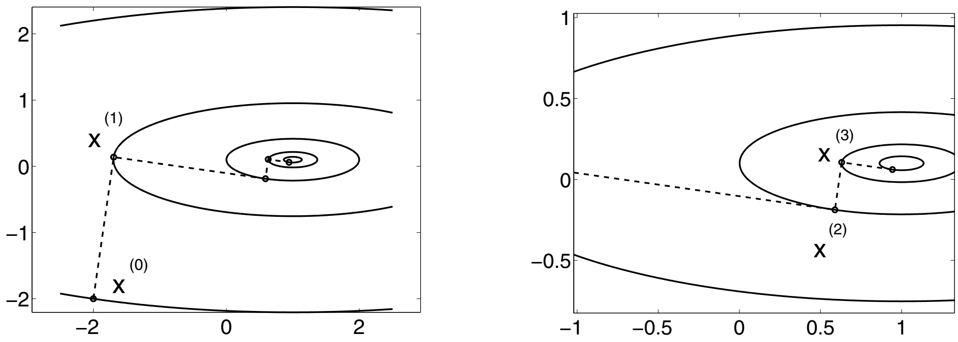


Gradient/Steepest Descent Method

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

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

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



- Exercise 1.8: 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,

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

- Exercise 1.9: 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 $k = 0, 1, \ldots$

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

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

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

until convergence

Theorem 1.15: Convergence

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

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