

10.4 Steepest Descent Methods

Recall : Newton \rightarrow Quadratic convergence
 Quasi-Newton \rightarrow Superlinear convergence

However, those depend on a good initial guess
 (If initial guess is bad, method might not converge!)

Today : Consider a method which converges independent of the initial guess .

Given $F: \mathbb{R}^n \rightarrow \mathbb{R}^n$, the solution to the system can be treated as the minimizer of the optimization problem :

$$F(\vec{x}^*) = 0 \Leftrightarrow \vec{x}^* = \operatorname{argmin}_{\vec{x} \in \mathbb{R}^n} g(\vec{x})$$

$$\text{where } g(\vec{x}) = \|F(\vec{x})\|^2 = \sum_{i=1}^h f_i^2(\vec{x})$$

Def. For $g: \mathbb{R}^n \rightarrow \mathbb{R}$, the gradient of g at $\vec{x} \in \mathbb{R}^n$, denoted by $\nabla g(\vec{x})$, is defined by

$$\nabla g(\vec{x}) = \begin{bmatrix} \frac{\partial g}{\partial x_1}(\vec{x}) \\ \vdots \\ \frac{\partial g}{\partial x_n}(\vec{x}) \end{bmatrix} \in \mathbb{R}^n$$

The **directional derivative** of g at \vec{x} in the direction $\vec{v} \in \mathbb{R}^n$ ($\|\vec{v}\|_2 = 1$) is defined by

$$D_{\vec{v}} g(\vec{x}) = \lim_{h \rightarrow 0} \frac{g(\vec{x} + h\vec{v}) - g(\vec{x})}{h} = \vec{v}^\top \cdot \nabla g(\vec{x})$$

Rmk. $D_{\vec{v}} g(\vec{x})$ describes the rate of change of g in the direction of \vec{v} .

Ex. If $g: \mathbb{R}^n \rightarrow \mathbb{R}$ is differentiable, show that $-\nabla g(\vec{x})$ is the direction of steepest descent in the value g at \vec{x} .

Pf. Let \vec{v} be a unit vector. Want to find direction \vec{v} that minimizes $\nabla g(\vec{x})^\top \vec{v}$.

$$\begin{aligned} \nabla g(\vec{x})^\top \vec{v} &= \|\nabla g(\vec{x})\| \|\vec{v}\| \cos(\theta) \\ &= \|\nabla g(\vec{x})\| \cos(\theta) \end{aligned}$$

\Rightarrow max occurs at $\theta = 0$

min occurs at $\theta = \pi$

$\Rightarrow \nabla g(\vec{x})$ points in direction of steepest descent

$-\nabla g(\vec{x})$ points in direction of steepest descent

Ex. Let $F(\vec{x}) = A\vec{x} + \vec{b}$. Then finding the root of F can be transformed into finding the minimum of $g(\vec{x}) = \|F(\vec{x})\|^2 = F(\vec{x})^T F(\vec{x})$, and $\nabla g(\vec{x}) = 2J_F(\vec{x}) \cdot F(\vec{x})$, where $J_F(\vec{x})$ is Jacobian of F .

More specifically,

$$\begin{aligned} g(\vec{x}) &= \|A\vec{x} - \vec{b}\|_2^2 = (\vec{x}^T A^T - \vec{b}^T)(A\vec{x} - \vec{b}) \\ &= \vec{x}^T A^T A \vec{x} - 2\vec{x}^T A^T \vec{b} + \vec{b}^T \vec{b} \end{aligned}$$

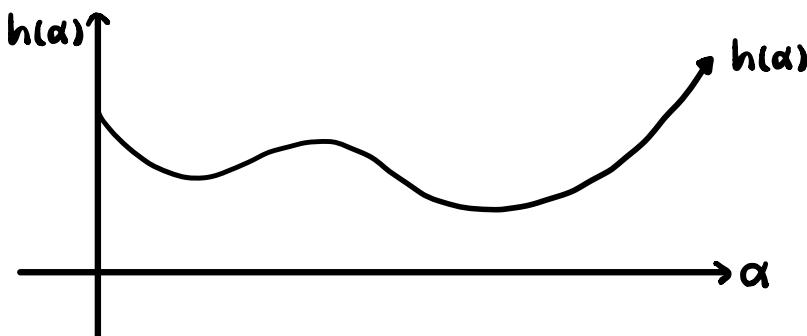
$$\nabla g(\vec{x}) = 2A^T A \vec{x} - 2A^T \vec{b} = 2A^T (A\vec{x} - \vec{b})$$

In the SD algorithm, update \vec{x} as follows :

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} - \alpha \nabla g(\vec{x}^{(k)})$$

where $\alpha > 0$ is a step size determined by minimizing the single-variable function

$$h(\alpha) = g(\vec{x}^{(k)} - \alpha \nabla g(\vec{x}^{(k)}))$$



Algorithm for SD

Given $\vec{x}^{(0)}$

For $k = 0, 1, \dots$:

1. Find steepest descent direction of g at $\vec{x}^{(k)}$ $(-\nabla g(\vec{x}^{(k)})$)
2. Determine $\hat{\alpha} > 0$ which is / approximates the solution to $\hat{\alpha} = \underset{\alpha}{\operatorname{argmin}} g(\vec{x}^{(k)} - \alpha \nabla g(\vec{x}^{(k)}))$
3. Update the solution $\vec{x}^{(k+1)} = \vec{x}^{(k)} - \hat{\alpha} \nabla g(\vec{x}^{(k)})$

Rmk. 1. No need to invert Jacobian

(at most $O(n^2)$ per iteration)

2. Minimizing $h(\alpha)$ at each iteration can be expensive!

Instead, choose 3 numbers $\alpha_1 < \alpha_2 < \alpha_3$ and minimize a quadratic polynomial $p(\alpha)$ that interpolates h at $\alpha_1, \alpha_2, \alpha_3$.

To choose $\alpha_1, \alpha_2, \alpha_3$, use backtracking:

- choose $\alpha_1 = 0, \alpha_3 = 1$
- if $h(\alpha_3) > h(\alpha_1)$, set $\alpha_3 \leftarrow \frac{\alpha_2}{2}$ until $h(\alpha_3) < h(\alpha_1)$
- finally, choose $\alpha_2 = \frac{\alpha_3}{2}$

9.1-9.2 Eigenvalues, Orthonormal Matrices, and Similarity Transformations

Def. Let $A \in \mathbb{R}^{n \times n}$, λ is called an **eigenvalue** of A if there exists $\vec{x} \in \mathbb{R}^n$ ($\vec{x} \neq 0$) such that $A\vec{x} = \lambda\vec{x}$. \vec{x} is the **eigenvector** corresponding to λ .

Define the **characteristic polynomial** of A as:

$$P_A(\lambda) = \det(A - \lambda I)$$

The eigenvalues are the roots of $P_A(\lambda)$.

The kernel of $A - \lambda I$ is called the **eigenspace** associated with λ , denoted by $E\lambda$:

$$E\lambda = \ker(A - \lambda I) = \{\vec{v} \in \mathbb{R}^n : A\vec{v} = \lambda\vec{v}\}$$

Eigenbasis: basis of A containing all linearly independent eigenvectors of A .

The dimension of $E\lambda$ is the **geometric multiplicity** of λ . The multiplicity of the root of $P_A(\lambda)$ is the **algebraic multiplicity**.

Rmk. 1. For $A \in \mathbb{R}^{n \times n}$, $\text{geom}(\lambda) \leq \text{alg}(\lambda)$
 2. $\text{geom}(\lambda) = \text{number of linearly independent eigenvectors of } A \text{ associated with } \lambda$.

Ex. Let D be upper-triangular matrix.
 Find all eigenvalues of D .

Sol. Since $P_D(\lambda) = \prod_{i=1}^n (d_{ii} - \lambda) \Rightarrow d_{ii} = \lambda$.

Def. A matrix $Q \in \mathbb{R}^{n \times n}$ is **orthogonal** if its column vectors form an ON basis in \mathbb{R}^n .

Thm. 9.10 Suppose Q is an orthogonal $n \times n$ matrix.

Then (i) Q is invertible with $Q^{-1} = Q^T$.

(ii) For any $\vec{x}, \vec{y} \in \mathbb{R}^n$, $(Q\vec{x})^T(Q\vec{y}) = \vec{x}^T\vec{y}$
 (angle preserving)

(iii) For any $\vec{x} \in \mathbb{R}^n$, $\|Q\vec{x}\|_2 = \|\vec{x}\|_2$
 (norm preserving)

Rmk. The converse of (i) holds:

$$Q^{-1} = Q^T \Rightarrow Q \text{ orthogonal}$$

Ex. The rotation matrix (CCW)

$$R = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \text{ is ON.}$$

Def. Two matrices are **similar** if nonsingular matrix exists with $A = S^{-1}BS$.

The map $B \mapsto S^{-1}BS$ is called a **similarity transformation** of B .

Thm. If A and B are similar with $A = S^{-1}BS$ and λ is an eigenvalue of A with associated eigenvector \vec{x} , then λ is an eigenvalue of B with associated eigenvector $S\vec{x}$.

Pf. By assumption, we have:

$$\begin{aligned} A\vec{x} &= \lambda\vec{x} \Rightarrow S^{-1}BS\vec{x} = \lambda\vec{x} \\ &\Rightarrow B(S\vec{x}) = \lambda(S\vec{x}) \quad \blacksquare \end{aligned}$$

Def. If $A \in \mathbb{R}^{n \times n}$ is similar to a diagonal matrix $D \in \mathbb{R}^{n \times n}$, there exists a nonsingular matrix $U \in \mathbb{C}^{n \times n}$ s.t.

$$T = U^{-1}AU$$

is an upper-triangular matrix whose diagonal matrix D and an ON matrix Q s.t.

$$A = QDQ^T$$

Rmk. $A \in \mathbb{C}^{n \times n}$ is **Hermitian** if $A = A^*$, where A^* is the conjugate transpose of A .
(MATLAB: "A'")

Fact 1. $A \in \mathbb{R}^{n \times n}$ symmetric \Rightarrow all $\lambda \in \mathbb{R}$
2. A symmetric is positive definite \Leftrightarrow all $\lambda > 0$.

9.3 The Power Method

Def. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of $A \in \mathbb{R}^{n \times n}$.

λ_1 is the **dominant eigenvalue** of A if

$$|\lambda_1| > |\lambda_i|, \quad i=2,3,\dots,n$$

Rmk. Not every matrix has dominant eigenvalue.

Goal: Approximate the dominant eigenvalue.

Assume that A has eigenvalues λ_i

satisfying $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ with associated eigenbasis $\{\vec{v}_i\}_{i=1}^n$.

Since \vec{v}_i are linearly independent, $\vec{x} \neq 0$ can be represented

$$\begin{aligned}\vec{x} &= a_1 \vec{v}_1 + a_2 \vec{v}_2 + \dots + a_n \vec{v}_n \\ \Rightarrow A^k \vec{x} &= A^k(a_1 \vec{v}_1 + a_2 \vec{v}_2 + \dots + a_n \vec{v}_n) \\ &= a_1 \lambda_1^k \vec{v}_1 + a_2 \lambda_2^k \vec{v}_2 + \dots + a_n \lambda_n^k \vec{v}_n \\ &= \lambda_1^k [a_1 \vec{v}_1 + a_2 \left(\frac{\lambda_2}{\lambda_1}\right)^k \vec{v}_2 + \dots + a_n \left(\frac{\lambda_n}{\lambda_1}\right)^k \vec{v}_n]\end{aligned}$$

Therefore, $\lim_{k \rightarrow \infty} A^k \vec{x} = \lim_{k \rightarrow \infty} \lambda_1^k a_1 \vec{v}_1$.

Thm. If \vec{v} is an eigenvector of A , then its corresponding eigenvalue is given by

$$\lambda = \frac{\vec{v}^T A \vec{v}}{\vec{v}^T \vec{v}}$$

called the Rayleigh Quotient

Pf. $A\vec{v} = \lambda \vec{v} \Rightarrow \vec{v}^T A \vec{v} = \lambda \vec{v}^T \vec{v}$

$$\Rightarrow \lambda = \frac{\vec{v}^T A \vec{v}}{\vec{v}^T \vec{v}}$$