ECE276A: Sensing & Estimation in Robotics Lecture 3: Unconstrained Optimization

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Field

- A field is a set F with two binary operations, + : F × F → F (addition) and · : F × F → F (multiplication), which satisfy the following axioms:
 - ▶ Associativity: a + (b + c) = (a + b) + c and a(bc) = (ab)c, $\forall a, b, c \in F$
 - Commutativity: a + b = b + a and ab = ba, $\forall a, b \in F$
 - ▶ Identity: $\exists 1, 0 \in F$ such that a + 0 = a and a1 = a, $\forall a \in F$
 - ▶ Inverse: $\forall a \in F, \exists -a \in F$ such that a + (-a) = 0 $\forall a \in F \setminus \{0\}, \exists a^{-1} \in F \setminus \{0\}$ such that $aa^{-1} = 1$
 - ▶ Distributivity: a(b + c) = (ab) + (ac), $\forall a, b, c \in F$

Examples: real numbers \mathbb{R} , complex numbers \mathbb{C} , rational numbers \mathbb{Q}

Vector Space

- A vector space over a field F is a set V with two binary operations, + : V × V → V (addition) and · : F × V → V (scalar multiplication), which satisfy the following axioms:
 - Associativity: $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}, \ \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V$
 - Compatibility: $a(b\mathbf{x}) = (ab)\mathbf{x}, \forall a, b \in F$ and $\forall \mathbf{x} \in V$
 - Commutativity: $\mathbf{x} + \mathbf{y} = \mathbf{x} + \mathbf{y}, \ \forall \mathbf{x}, \mathbf{y} \in V$
 - Identity: $\exists \mathbf{0} \in V$ and $1 \in F$ such that $\mathbf{x} + \mathbf{0} = \mathbf{x}$ and $1\mathbf{x} = \mathbf{x}$, $\forall \mathbf{x} \in V$
 - Inverse: $\forall x \in V, \exists -x \in V \text{ such that } x + (-x) = \mathbf{0}$
 - ▶ Distributivity: $a(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + b\mathbf{y}$ and $(a + b)\mathbf{x} = a\mathbf{x} + b\mathbf{x}$, $\forall a, b \in F$ and $\forall \mathbf{x}, \mathbf{y} \in V$
- Examples: real vectors ℝ^d, complex vectors ℂ^d, rational vectors ℚ^d, functions ℝ^d → ℝ

Basis and Dimension

- A **basis** of a vector space V over a field F is a set $B \subseteq V$ that satisfies:
 - ▶ linear independence: for all finite $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \subseteq B$, if $a_1\mathbf{x}_1 + \cdots + a_m\mathbf{x}_m = 0$ for some $a_1, \ldots, a_m \in F$, then $a_1 = \cdots = a_m = 0$
 - ▶ B spans V: $\forall \mathbf{x} \in V$, $\exists \mathbf{x}_1, \dots, \mathbf{x}_d \in B$ and unique $a_1, \dots, a_d \in F$ such that $\mathbf{x} = a_1 \mathbf{x}_1 + \dots + a_d \mathbf{x}_d$

The dimension d of a vector space V is the cardinality of its bases

Inner Product and Norm

An inner product on a vector space V over a field F is a function $\langle \cdot, \cdot \rangle : V \times V \mapsto F$ such that for all $a \in F$ and all $\mathbf{x}, \mathbf{y}, \mathbf{z} \in V$:

$$\blacktriangleright \langle a\mathbf{x}, \mathbf{y} \rangle = a \langle \mathbf{x}, \mathbf{y} \rangle \qquad (\text{homogeneity})$$

- $\langle \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle$ (additivity)
- $\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\langle \mathbf{y}, \mathbf{x} \rangle}$ (conjugate symmetry) $\langle \mathbf{x}, \mathbf{x} \rangle \ge 0$ (non-negativity)

A norm on a vector space V over a field F is a function || · || : V → ℝ such that for all a ∈ F and all x, y ∈ V:

 $||a\mathbf{x}|| = |a|||\mathbf{x}||$ (absolute homogeneity)

$$||\mathbf{x} + \mathbf{y}|| \le ||\mathbf{x}|| + ||\mathbf{y}||$$
 (triangle inequality)

- $||\mathbf{x}|| = 0 \text{ iff } \mathbf{x} = 0$ (definiteness)

Euclidean Vector Space

- ► A Euclidean vector space ℝ^d is a vector space with finite dimension d over the real numbers ℝ
- A Euclidean vector x ∈ ℝ^d is a collection of scalars x_i ∈ ℝ for i = 1,..., d organized as a column:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

• The **transpose** of $\mathbf{x} \in \mathbb{R}^d$ is organized as a row: $\mathbf{x}^{\top} = \begin{bmatrix} x_1 & \cdots & x_d \end{bmatrix}$

▶ The Euclidean inner product between two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ is:

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y} = \sum_{i=1}^d x_i y_i$$

► The Euclidean norm of a vector $\mathbf{x} \in \mathbb{R}^d$ is $\|\mathbf{x}\|_2 := \sqrt{\mathbf{x}^\top \mathbf{x}}$ and satisfies: $\max_{1 \le i \le d} |x_i| \le \|\mathbf{x}\|_2 \le \sqrt{d} \max_{1 \le i \le d} |x_i|$ $\|\mathbf{x}^\top \mathbf{y}\| < \|\mathbf{x}\|_2 \|\mathbf{y}\|_2$ (Cauchy-Schwarz Inequality)

Matrices

▶ A matrix $A \in \mathbb{R}^{m \times n}$ is a rectangular array of scalars $A_{ij} \in \mathbb{R}$ for i = 1, ..., m and j = 1, ..., n

- ▶ The entries of the **transpose** $A^{\top} \in \mathbb{R}^{n \times m}$ of a matrix $A \in \mathbb{R}^{m \times n}$ are $A_{ij}^{\top} = A_{ji}$. The transpose satisfies: $(AB)^{\top} = B^{\top}A^{\top}$
- The **trace** of a matrix $A \in \mathbb{R}^{n \times n}$ is the sum of its diagonal entries:

$$tr(A) := \sum_{i=1}^{n} A_{ii} \qquad tr(ABC) = tr(BCA) = tr(CAB)$$

▶ The **Frobenius inner product** between two matrices $X, Y \in \mathbb{R}^{m \times n}$ is:

$$\langle X, Y \rangle = \operatorname{tr}(X^{\top}Y)$$

► The **Frobenius norm** of a matrix $X \in \mathbb{R}^{m \times n}$ is: $\|X\|_F := \sqrt{\operatorname{tr}(X^\top X)}$

Matrix Determinant and Inverse

• The **determinant** of a matrix $A \in \mathbb{R}^{n \times n}$ is:

$$\det(A) := \sum_{j=1}^n A_{ij} \mathbf{cof}_{ij}(A)$$
 $\det(AB) = \det(A) \det(B) = \det(BA)$

where $\mathbf{cof}_{ij}(A)$ is the **cofactor** of the entry A_{ij} and is equal to $(-1)^{i+j}$ times the determinant of the $(n-1) \times (n-1)$ submatrix that results when the *i*th-row and *j*th-col of A are removed. This recursive definition uses the fact that the determinant of a scalar is the scalar itself.

The adjugate is the transpose of the cofactor matrix:

$$\operatorname{adj}(A) := \operatorname{cof}(A)^{\top}$$

• The **inverse** A^{-1} of A exists iff det $(A) \neq 0$ and satisfies:

$$A^{-1} = \frac{\operatorname{adj}(A)}{\det(A)}$$
 $(AB)^{-1} = B^{-1}A^{-1}$

Matrix Inversion Lemma

Square completion:

$$\frac{1}{2}x^{\top}Ax + b^{\top}x + c = \frac{1}{2}(x + A^{-1}b)^{\top}A(x + A^{-1}b) + c - \frac{1}{2}b^{\top}A^{-1}b$$

Woodbury matrix identity:

$$(A + BDC)^{-1} = A^{-1} - A^{-1}B(CA^{-1}B + D^{-1})^{-1}CA^{-1}$$

Block matrix inversion:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} I & 0 \\ D^{-1}C & I \end{bmatrix}^{-1} \begin{bmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{bmatrix}^{-1} \begin{bmatrix} I & BD^{-1} \\ 0 & I \end{bmatrix}^{-1}$$
$$= \begin{bmatrix} I & 0 \\ -D^{-1}C & I \end{bmatrix} \begin{bmatrix} (A - BD^{-1}C)^{-1} & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} I & -BD^{-1} \\ 0 & I \end{bmatrix}$$
$$= \begin{bmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C (A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C (A - BD^{-1}C)^{-1}BD^{-1} \end{bmatrix}$$

Eigenvalue Decomposition

▶ For any $A \in \mathbb{R}^{n \times n}$, if there exists $\mathbf{q} \in \mathbb{C}^n \setminus {\mathbf{0}}$ and $\lambda \in \mathbb{C}$ such that:

 $A\mathbf{q} = \lambda \mathbf{q}$

then **q** is an **eigenvector** corresponding to the **eigenvalue** λ .

- A real matrix can have complex eigenvalues and eigenvectors, which appear in conjugate pairs.
- ► Eigenvectors are not unique since for any c ∈ C \ {0}, cq is an eigenvector corresponding to the same eigenvalue.
- ▶ The *n* eigenvalues of $A \in \mathbb{R}^{n \times n}$ are precisely the *n* roots of the **characteristic polynomial** of *A*:

$$p(\lambda) := \det(\lambda I - A)$$

We can put all *n* equations Aq_i = λ_iq_i to obtain the eigen decomposition of A:

$$A = Q \Lambda Q^{-1}$$

Eigenvalue Decomposition

The roots of a polynomial are continuous functions of its coefficients and hence the eigenvalues of a matrix are continuous functions of its entries.

$$\operatorname{tr}(A) := \sum_{i=1}^{n} \lambda_i$$
 $\operatorname{det}(A) := \prod_{i=1}^{n} \lambda_i$

• A^{\top} has the same eigenvalues and eigenvectors as A

- $A^{\top}A$ has the same eigenvectors as A but its eigenvalues are λ^2
- A^k for k = 1, 2, ... has the same eigenvectors as A but its eigenvalues are λ^k
- A^{-1} has the same eigenvectors as A but its eigenvalues are λ^{-1}
- The eigenvalues of A are invariant under any unitary transform U*AU for U*U = UU* = I
- If A is symmetric (A^T = A), then all its eigenvalues are real and all its eigenvectors are orthogonal (Q⁻¹ = Q^T)

Singular Value Decomposition

- An eigen-decomposition does not exist for $A \in \mathbb{R}^{m \times n}$
- A ∈ ℝ^{m×n} with rank r ≤ min {m, n} can be diagonalized by two orthogonal matrices U ∈ ℝ^{m×m} and V ∈ ℝ^{n×n} via singular value decomposition:

$$A = U\Sigma V^{\top} \qquad \Sigma = \begin{bmatrix} & \ddots & \\ & \sigma_r \end{bmatrix} \in \mathbb{R}^{m \times n}$$

- *U* contains the *m* orthogonal eigenvectors of the symmetric matrix $AA^{\top} \in \mathbb{R}^{m \times m}$ and satisfies $U^{\top}U = UU^{\top} = I$
- ▶ *V* contains the *n* orthogonal eigenvectors of the symmetric matrix $A^{\top}A \in \mathbb{R}^{n \times n}$ and satisfies $V^{\top}V = VV^{\top} = I$
- Σ contains the singular values σ_i = √λ_i, equal to the square roots of the *r* non-zero eigenvalues λ_i of AA^T or A^TA, on its diagonal
- If A is normal (A^TA = AA^T), its singular values are related to its eigenvalues via σ_i = |λ_i|

Matrix Pseudo Inverse

The pseudo-inverse A[†] ∈ ℝ^{n×m} of A ∈ ℝ^{m×n} can be obtained from its SVD A = UΣV[⊤]:

$$\mathcal{A}^{\dagger} = \mathcal{V}\Sigma^{\dagger}\mathcal{U}^{\mathcal{T}} \qquad \Sigma^{\dagger} = \begin{bmatrix} 1/\sigma_{1} & & & \\ & \ddots & & \\ & & 1/\sigma_{r} & \end{bmatrix} \in \mathbb{R}^{n imes m}$$

▶ The pseudo-inverse $A^{\dagger} \in \mathbb{R}^{n \times m}$ satisfies the Moore-Penrose conditions:

$$AA^{\dagger}A = A$$

$$A^{\dagger}AA^{\dagger} = A^{\dagger}$$

$$(AA^{\dagger})^{\top} = AA^{\dagger}$$

$$(A^{\dagger}A)^{\top} = A^{\dagger}A$$

Linear System of Equations

- Consider the linear system of equations $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$, and $A \in \mathbb{R}^{m \times n}$ with SVD $A = U\Sigma V^{\top}$ and rank r
- The column space or image of A is im(A) ⊆ ℝ^m and is spanned by the r columns of U corresponding to non-zero singular values
- The null space or kernel of A is ker(A) ⊆ ℝⁿ and is spanned by the n − r columns of V corresponding to zero singular values
- The row space or co-image of A is im(A^T) ⊆ ℝⁿ and is spanned by the r columns of V corresponding to non-zero singular values
- The left null space or co-kernel of A is ker(A^T) ⊆ ℝ^m and is spanned by the m − r columns of U corresponding to zero singular values
- The **domain** of A is $\mathbb{R}^n = ker(A) \oplus im(A^{\top})$
- The **co-domain** of A is $\mathbb{R}^m = ker(A^{\top}) \oplus im(A)$

Solution of Linear System of Equations

- Consider the linear system of equations $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$, and $A \in \mathbb{R}^{m \times n}$ with SVD $A = U\Sigma V^{\top}$ and rank r
- If b ∈ im(A), i.e., b^Tv = 0 for all v ∈ ker(A^T), then Ax = b has one or infinitely many solutions x = A[†]b + (I − A[†]A)y for any y ∈ ℝⁿ
- If b ∉ im(A), then no solution exists and x = A[†]b is an approximate solution with minimum ||x|| and ||Ax b|| norms

• If m = n = r, then $A\mathbf{x} = \mathbf{b}$ has a unique solution $\mathbf{x} = A^{\dagger}\mathbf{b} = A^{-1}\mathbf{b}$

Positive Semidefinite Matrices

The product x^TAx for A ∈ ℝ^{n×n} and x ∈ ℝⁿ is called a quadratic form and A can be assumed symmetric, A = A^T, because:

$$\frac{1}{2}\mathbf{x}^{\top}(\mathbf{A} + \mathbf{A}^{\top})\mathbf{x} = \mathbf{x}^{\top}\mathbf{A}\mathbf{x}, \qquad \forall \mathbf{x} \in \mathbb{R}^{n}$$

- A symmetric matrix A ∈ ℝ^{n×n} is positive semidefinite if x^TAx ≥ 0 for all x ∈ ℝⁿ.
- A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is **positive definite** if it is positive semidefinite and if $\mathbf{x}^{\top} A \mathbf{x} = 0$ implies $\mathbf{x} = 0$.
- All eigenvalues of a symmetric positive semidefinite matrix are non-negative.
- All eigenvalues of a symmetric positive definite matrix are positive.

Schur Complement

• The Schur complement of block *D* of $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ is $S_D = A - BD^{-1}C$

• The Schur complement of block A of $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ is $S_A = D - CA^{-1}B$

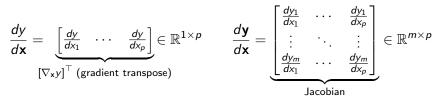
▶ Let
$$M = \begin{bmatrix} A & B \\ B^{\top} & D \end{bmatrix}$$
 be symmetric. Then:
▶ $M \succ 0 \Leftrightarrow A \succ 0, S_A = D - B^{\top}A^{-1}B \succ 0$
▶ $M \succ 0 \Leftrightarrow D \succ 0, S_D = A - BD^{-1}B^{\top} \succ 0$
▶ $M \succeq 0 \Leftrightarrow A \succeq 0, S_A \succeq 0, (I - AA^{\dagger})B = 0$
▶ $M \succeq 0 \Leftrightarrow D \succeq 0, S_D \succeq 0, (I - DD^{\dagger})B^{\top} = 0$

Derivatives (numerator layout)

• Derivatives of $\mathbf{y} \in \mathbb{R}^m$ and $\mathbf{Y} \in \mathbb{R}^{m \times n}$ by scalar $x \in \mathbb{R}$:

$$\frac{d\mathbf{y}}{dx} = \begin{bmatrix} \frac{dy_1}{dx} \\ \vdots \\ \frac{dy_m}{dx} \end{bmatrix} \in \mathbb{R}^{m \times 1} \qquad \frac{dY}{dx} = \begin{bmatrix} \frac{dY_{11}}{dx} & \cdots & \frac{dY_{1n}}{dx} \\ \vdots & \ddots & \vdots \\ \frac{dY_{m1}}{dx} & \cdots & \frac{dY_{mn}}{dx} \end{bmatrix} \in \mathbb{R}^{m \times n}$$

• Derivatives of $y \in \mathbb{R}$ and $\mathbf{y} \in \mathbb{R}^m$ by vector $\mathbf{x} \in \mathbb{R}^p$:



• Derivative of $y \in \mathbb{R}$ by matrix $\mathbf{X} \in \mathbb{R}^{p \times q}$:

$$\frac{dy}{dX} = \begin{bmatrix} \frac{dy}{dX_{11}} & \cdots & \frac{dy}{dX_{p1}} \\ \vdots & \ddots & \vdots \\ \frac{dy}{dX_{1q}} & \cdots & \frac{dy}{dX_{pq}} \end{bmatrix} \in \mathbb{R}^{q \times p}$$

Matrix Derivatives Example

$$\blacktriangleright \ \frac{d}{dX_{ij}}X = \mathbf{e}_i\mathbf{e}_j^{\top}$$

$$\quad \bullet \quad \frac{d}{d\mathbf{x}}A\mathbf{x} = A$$

$$\quad \quad \frac{d}{d\mathbf{x}}\mathbf{x}^{\top}A\mathbf{x} = \mathbf{x}^{\top}(A + A^{\top})$$

•
$$\frac{d}{dx}M^{-1}(x) = -M^{-1}(x)\frac{dM(x)}{dx}M^{-1}(x)$$

$$\quad \bullet \quad \frac{d}{dX} \operatorname{tr}(AX^{-1}B) = -X^{-1}BAX^{-1}$$

•
$$\frac{d}{dX} \log \det X = X^{-1}$$

Matrix Derivatives Example

$$\frac{d}{d\mathbf{x}}A\mathbf{x} = \begin{bmatrix} \frac{d}{dx_1}\sum_{j=1}^n A_{1j}x_j & \cdots & \frac{d}{dx_n}\sum_{j=1}^n A_{1j}x_j \\ \vdots & \ddots & \vdots \\ \frac{d}{dx_1}\sum_{j=1}^n A_{mj}x_j & \cdots & \frac{d}{dx_n}\sum_{j=1}^n A_{mj}x_j \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{bmatrix}$$

$$\frac{d}{d\mathbf{x}}\mathbf{x}^\top A\mathbf{x} = \mathbf{x}^\top A^\top \frac{d\mathbf{x}}{d\mathbf{x}} + \mathbf{x}^\top \frac{dA\mathbf{x}}{d\mathbf{x}} = \mathbf{x}^\top (A^\top + A)$$

$$M(x)M^{-1}(x) = I \quad \Rightarrow \quad 0 = \begin{bmatrix} \frac{d}{dx}M(x) \end{bmatrix} M^{-1}(x) + M(x) \begin{bmatrix} \frac{d}{dx}M^{-1}(x) \end{bmatrix}$$

$$\frac{d}{dX_{ij}} \operatorname{tr}(AX^{-1}B) = \operatorname{tr}(A\frac{d}{dX_{ij}}X^{-1}B) = -\operatorname{tr}(AX^{-1}\mathbf{e}_i\mathbf{e}_j^\top X^{-1}B)$$

$$= -\mathbf{e}_j^\top X^{-1}BAX^{-1}\mathbf{e}_i = -\mathbf{e}_i^\top (X^{-1}BAX^{-1})^\top \mathbf{e}_j$$

$$\frac{d}{dX_{ij}} \log \det X = \frac{1}{\det(X)} \frac{d}{dX_{ij}} \sum_{k=1}^n X_{ik} \operatorname{cof}_{ik}(X)$$

$$= \frac{1}{\det(X)} \mathbf{cof}_{ij}(X) = \frac{1}{\det(X)} \mathbf{adj}_{ji}(X) = \mathbf{e}_i^\top X^{-T} \mathbf{e}_j$$

Unconstrained Optimization

Many problems we encounter in this course, lead to an unconstrained optimization problem over the Euclidean vector space R^d:

$$\min_{\mathbf{x}\in\mathbb{R}^d}f(\mathbf{x})$$

- A global minimizer $\mathbf{x}^* \in \mathbb{R}^d$ satisfies $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^d$. The value $f(\mathbf{x}^*)$ is called global minimum.
- ▶ A local minimizer $\mathbf{x}^* \in \mathbb{R}^d$ satisfies $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{N}(\mathbf{x}^*)$, where $\mathcal{N}(\mathbf{x}^*) \subset \mathbb{R}^d$ is a neighborhood around \mathbf{x}^* (e.g., an open ball with small radius centered at \mathbf{x}^*). The value $f(\mathbf{x}^*)$ is called local minimum.
- ▶ The objective function $f : \mathbb{R}^d \mapsto \mathbb{R}$ is **differentiable** if the gradient:

$$abla f(\mathbf{x}) := \begin{bmatrix} rac{\partial f(\mathbf{x})}{\partial x_1} & \cdots & rac{\partial f(\mathbf{x})}{\partial x_d} \end{bmatrix}^\top \in \mathbb{R}^d$$

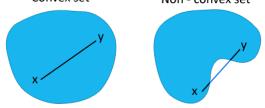
exists at each $\mathbf{x} \in \mathbb{R}^d$

- A critical point $\bar{\mathbf{x}} \in \mathbb{R}^d$ satisfies $\nabla f(\bar{\mathbf{x}}) = 0$ or $\nabla f(\bar{\mathbf{x}}) =$ undefined
- All minimizers are critical points but not all critical points are minimizers. A critical point is either a local maximizer, a local minimizer, or neither (saddle point).

Convexity

▶ A set $\mathcal{D} \subseteq \mathbb{R}^d$ is **convex** if $\lambda \mathbf{x} + (1 - \lambda)\mathbf{y} \in \mathcal{D}$ for all $\mathbf{x}, \mathbf{y} \in \mathcal{D}$, $\lambda \in [0, 1]$

A convex set contains the line segment between any two points in it Convex set
Non - convex set



- A function $f : \mathcal{D} \mapsto \mathbb{R}$ with $\mathcal{D} \subseteq \mathbb{R}^d$ is **convex** if:
 - D is a convex set
 - ► $f(\lambda \mathbf{x} + (1 \lambda)\mathbf{y}) \le \lambda f(\mathbf{x}) + (1 \lambda)f(\mathbf{y})$ for all $\mathbf{x}, \mathbf{y} \in \mathcal{D}$, $\lambda \in [0, 1]$
- First-order convexity condition: a differentiable f : D → R with convex D is convex iff f(y) ≥ f(x) + ∇f(x)^T(y x) for all x, y ∈ D
- Second-order convexity condition: a twice-differentiable $f : \mathcal{D} \mapsto \mathbb{R}$ with convex \mathcal{D} is convex iff $\nabla^2 f(\mathbf{x}) \succeq 0$ for all $\mathbf{x} \in \mathcal{D}$

Descent Direction

Consider the **unconstrained optimization problem**:

 $\min_{\mathbf{x}\in\mathbb{R}^d}f(\mathbf{x})$

Descent Direction Theorem

Suppose f is differentiable at $\mathbf{\bar{x}}$. If $\exists \delta \mathbf{x}$ such that $\nabla f(\mathbf{\bar{x}})^{\top} \delta \mathbf{x} < 0$, then $\exists \epsilon > 0$ such that $f(\mathbf{\bar{x}} + \alpha \delta \mathbf{x}) < f(\mathbf{\bar{x}})$ for all $\alpha \in (0, \epsilon)$.

- The vector $\delta \mathbf{x}$ is called a **descent direction**
- The theorem states that if a descent direction exists at x
 , then it is possible to move to a new point that has a lower f value
- Steepest descent direction: $\delta \mathbf{x} := -\frac{\nabla f(\bar{\mathbf{x}})}{\|\nabla f(\bar{\mathbf{x}})\|}$
- Based on this theorem, we can derive conditions for determining the optimality of x

Optimality Conditions

First-order Necessary Condition

Suppose f is differentiable at $\bar{\mathbf{x}}$. If $\bar{\mathbf{x}}$ is a local minimizer, then $\nabla f(\bar{\mathbf{x}}) = 0$.

Second-order Necessary Condition

Suppose f is twice-differentiable at $\bar{\mathbf{x}}$. If $\bar{\mathbf{x}}$ is a local minimizer, then $\nabla f(\bar{\mathbf{x}}) = 0$ and $\nabla^2 f(\bar{\mathbf{x}}) \succeq 0$.

Second-order Sufficient Condition

Suppose f is twice-differentiable at $\bar{\mathbf{x}}$. If $\nabla f(\bar{\mathbf{x}}) = 0$ and $\nabla^2 f(\bar{\mathbf{x}}) \succ 0$, then $\bar{\mathbf{x}}$ is a local minimizer.

Necessary and Sufficient Condition

Suppose f is differentiable at $\bar{\mathbf{x}}$. If f is **convex**, then $\bar{\mathbf{x}}$ is a global minimizer **if and only if** $\nabla f(\bar{\mathbf{x}}) = 0$.

Descent Optimization Methods

- A critical point of f can be obtained by solving ∇f(x) = 0 but an explicit solution may be difficult to derive
- **Descent methods**: iterative methods to obtain a solution of $\nabla f(\mathbf{x}) = 0$
- Given an initial guess x^(k), take a step of size α^(k) > 0 along a descent direction δx^(k):

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}^{(k)}$$

- ▶ Different methods differ in the way $\delta \mathbf{x}^{(k)}$ and $\alpha^{(k)}$ are chosen
- $\delta \mathbf{x}^{(k)}$ needs to be a descent direction: $\nabla f(\mathbf{x}^{(k)})^{\top} \delta \mathbf{x}^{(k)} < 0$, $\forall \mathbf{x}^{(k)} \neq \mathbf{x}^{*}$
- - ▶ In practice, $\alpha^{(k)}$ is obtained via approximate line search methods

Gradient Descent (First-Order Method)

▶ Idea: $-\nabla f(\mathbf{x}^{(k)})$ points in the direction of steepest local descent

• Gradient descent: let $\delta \mathbf{x}^{(k)} := -\nabla f(\mathbf{x}^{(k)})$ and iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \nabla f(\mathbf{x}^{(k)})$$

Step size: a good choice for α^(k) is ¹/_L, where L > 0 is the Lipschitz constant of ∇f(x):

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{x}')\| \le L \|\mathbf{x} - \mathbf{x}'\| \qquad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$$

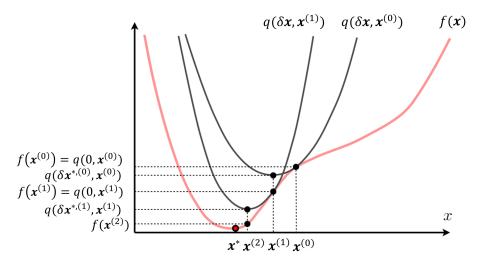
Newton's Method (Second-Order Method)

- Newton's method: iteratively approximates f by a quadratic function
- Since δx is a 'small' change to the initial guess x^(k), we can approximate f using a Taylor-series expansion:

$$f(\mathbf{x}^{(k)} + \delta \mathbf{x}) \approx f(\mathbf{x}^{(k)}) + \underbrace{\left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x} = \mathbf{x}^{(k)}}\right)}_{\text{Gradient Transpose}} \delta \mathbf{x} + \frac{1}{2} \delta \mathbf{x}^{\top} \underbrace{\left(\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}}\Big|_{\mathbf{x} = \mathbf{x}^{(k)}}\right)}_{\text{Hessian}} \delta \mathbf{x}$$
$$=: \underbrace{q(\delta \mathbf{x}, \mathbf{x}^{(k)})}_{\text{guadratic function in } \delta \mathbf{x}}$$

► The symmetric Hessian matrix ∇²f(x^(k)) needs to be positive-definite for this method to work.

Newton's Method (Second-Order Method)



Newton's Method (Second-Order Method)

- Find $\delta \mathbf{x}$ that minimizes the quadratic approximation to $f(\mathbf{x}^{(k)} + \delta \mathbf{x})$
- Since this is an unconstrained optimization problem, δx can be determined by setting the derivative with respect to δx to zero:

$$0 = \frac{\partial q(\delta \mathbf{x}, \mathbf{x}^{(k)})}{\partial \delta \mathbf{x}} = \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) + \delta \mathbf{x}^{\top} \left(\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)$$
$$\Rightarrow \quad \left(\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} = - \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)^{\top}$$

The above is a linear system of equations and can be solved when the Hessian is invertible, i.e., ∇²f(x^(k)) ≻ 0:

$$\delta \mathbf{x} = -\left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

Newton's method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \left[\nabla^2 f(\mathbf{x}^{(k)}) \right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

Newton's Method (Comments)

- Newton's method, like any other descent method, converges only to a local minimum
- Damped Newton phase: when the iterates are "far away" from the optimal point, the function value is decreased sublinearly, i.e., the step sizes α^(k) are small
- Quadratic convergence phase: when the iterates are "sufficiently close" to the optimum, full Newton steps are taken, i.e., α^(k) = 1, and the function value converges quadratically to the optimum
- A disadvantage of Newton's method is the need to form the Hessian, which can be numerically ill-conditioned or very computationally expensive in high-dimensional problems

Gauss-Newton's Method

Gauss-Newton is an approximation to Newton's method that avoids computing the Hessian. It is applicable when the objective function has the following quadratic form:

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{e}(\mathbf{x})^{\top} \mathbf{e}(\mathbf{x}) \qquad \mathbf{e}(\mathbf{x}) \in \mathbb{R}^{m}$$

► The Jacobian and Hessian matrices are:

Jacobian:

Hessian:

$$\begin{aligned} \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} &= \mathbf{e}(\mathbf{x}^{(k)})^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} \right) \\ \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} &= \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} \right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} \right) \\ &+ \sum_{i=1}^{m} e_i(\mathbf{x}^{(k)}) \left(\frac{\partial^2 e_i(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x}=\mathbf{x}^{(k)}} \right) \end{aligned}$$

Gauss-Newton's Method

Near the minimum of f, the second term in the Hessian is small relative to the first and the Hessian can be approximated according to:

$$\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}} \approx \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)$$

- The above does not involve any second derivatives
- Setting the gradient of this new quadratic approximation of f with respect to δx to zero, leads to the system:

$$\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

Gauss-Newton's method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}$$

Gauss-Newton's Method (Alternative Derivation)

Another way to think about the Gauss-Newton method is to start with a Taylor expansion of e(x) instead of f(x):

$$\mathbf{e}(\mathbf{x}^{(k)} + \delta \mathbf{x}) \approx \mathbf{e}(\mathbf{x}^{(k)}) + \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x} = \mathbf{x}^{(k)}}\right) \delta \mathbf{x}$$

Substituting into f leads to:

$$f(\mathbf{x}^{(k)} + \delta \mathbf{x}) \approx \frac{1}{2} \left(\mathbf{e}(\mathbf{x}^{(k)}) + \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} \right)^{\top} \left(\mathbf{e}(\mathbf{x}^{(k)}) + \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} \right)$$

• Minimizing this with respect to $\delta \mathbf{x}$ leads to the same system as before:

$$\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

Levenberg-Marquardt's Method

The Levenberg-Marquardt modification to the Gauss-Newton method uses a positive diagonal matrix D to condition the Hessian approximation:

$$\left(\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) + \lambda D\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

When λ ≥ 0 is large, the descent vector δx corresponds to a very small step in the direction of steepest descent. This helps when the Hessian approximation is poor or poorly conditioned by providing a meaningful direction.

Levenberg-Marquardt's Method (Summary)

> An iterative optimization approach for the unconstrained problem:

$$\min_{\mathbf{x}} f(\mathbf{x}) := \frac{1}{2} \sum_{j} \mathbf{e}_{j}(\mathbf{x})^{\top} \mathbf{e}_{j}(\mathbf{x}) \qquad \mathbf{e}_{j}(\mathbf{x}) \in \mathbb{R}^{m_{j}}, \ \mathbf{x} \in \mathbb{R}^{n_{j}}$$

• Given an initial guess $\mathbf{x}^{(k)}$, determine a descent direction $\delta \mathbf{x}$ by solving:

$$\left(\sum_{j} J_j(\mathbf{x}^{(k)})^\top J_j(\mathbf{x}^{(k)}) + \lambda D\right) \delta \mathbf{x} = -\left(\sum_{j} J_j(\mathbf{x}^{(k)})^\top \mathbf{e}_j(\mathbf{x}^{(k)})\right)$$

where $J_j(\mathbf{x}) := \frac{\partial \mathbf{e}_j(\mathbf{x})}{\partial \mathbf{x}} \in \mathbb{R}^{m_j \times n}$, $\lambda \ge 0$, $D \in \mathbb{R}^{n \times n}$ is a positive diagonal matrix, e.g., $D = \operatorname{diag}\left(\sum_j J_j(\mathbf{x}^{(k)})^\top J_j(\mathbf{x}^{(k)})\right)$

Obtain an updated estimate according to:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}$$

Unconstrained Optimization Example

• Let $f(\mathbf{x}) := \frac{1}{2} \sum_{j=1}^{n} \|A_j \mathbf{x} + b_j\|_2^2$ for $\mathbf{x} \in \mathbb{R}^d$ and assume $\sum_{j=1}^{n} A_j^\top A_j \succ 0$

Solve the unconstrained optimization problem min_x f(x) using:

- The necessary and sufficient optimality condition for convex function f
- Gradient descent
- Newton's method
- Gauss-Newton's method

• We will need $\nabla f(\mathbf{x})$ and $\nabla^2 f(\mathbf{x})$:

$$\frac{df(\mathbf{x})}{d\mathbf{x}} = \frac{1}{2} \sum_{j=1}^{n} \frac{d}{d\mathbf{x}} ||A_j \mathbf{x} + b_j||_2^2 = \sum_{j=1}^{n} (A_j \mathbf{x} + b_j)^\top A_j$$
$$\nabla f(\mathbf{x}) = \frac{df(\mathbf{x})}{d\mathbf{x}}^\top = \left(\sum_{j=1}^{n} A_j^\top A_j\right) \mathbf{x} + \left(\sum_{j=1}^{n} A_j^\top b_j\right)$$
$$\nabla^2 f(\mathbf{x}) = \frac{d}{d\mathbf{x}} \nabla f(\mathbf{x}) = \sum_{j=1}^{n} A_j^\top A_j \succ 0$$

Necessary and Sufficient Optimality Condition

Solve $\nabla f(\mathbf{x}) = 0$ for \mathbf{x} :

$$0 = \nabla f(\mathbf{x}) = \left(\sum_{j=1}^{n} A_j^{\top} A_j\right) \mathbf{x} + \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$
$$\mathbf{x} = -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

▶ The solution above is unique since we assumed that $\sum_{j=1}^{n} A_j^{\top} A_j \succ 0$

Gradient Descent

- Start with an initial guess x⁽⁰⁾ = 0
- At iteration k, gradient descent uses the descent direction δx^(k) = -∇f(x^(k))
- Given arbitary $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^d$, determine the Lipschitz constant of $\nabla f(\mathbf{x})$:

$$\|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\| = \left\| \left(\sum_{j=1}^n A_j^\top A_j \right) (\mathbf{x}_1 - \mathbf{x}_2) \right\| \le \underbrace{\left\| \sum_{j=1}^n A_j^\top A_j \right\|}_{L} \|\mathbf{x}_1 - \mathbf{x}_2\|$$

• Choose step size $\alpha^{(k)} = \frac{1}{L}$ and iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}^{(k)}$$
$$= \mathbf{x}^{(k)} - \frac{1}{L} \left(\sum_{j=1}^{n} A_j^{\top} A_j \right) \mathbf{x}^{(k)} - \frac{1}{L} \left(\sum_{j=1}^{n} A_j^{\top} b_j \right)$$

Newton's Method

• Start with an initial guess
$$\mathbf{x}^{(0)} = \mathbf{0}$$

▶ At iteration *k*, Newton's method uses the descent direction:

$$\delta \mathbf{x}^{(k)} = -\left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$$
$$= -\mathbf{x}^{(k)} - \left(\sum_{j=1}^n A_j^\top A_j\right)^{-1} \left(\sum_{j=1}^n A_j^\top b_j\right)$$

and updates the solution estimate via:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \delta \mathbf{x}^{(k)} = -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

Note that for this problem, Newton's method converges in one iteration!

Gauss-Newton's Method

- $f(\mathbf{x})$ is of the form $\frac{1}{2} \sum_{j=1}^{n} \mathbf{e}_j(\mathbf{x})^\top \mathbf{e}_j(\mathbf{x})$ for $\mathbf{e}_j(\mathbf{x}) := A_j \mathbf{x} + b_j$
- The Jacobian of $\mathbf{e}_j(\mathbf{x})$ is $J_j(\mathbf{x}) = A_j$
- Start with an initial guess $\mathbf{x}^{(0)} = \mathbf{0}$
- At iteration k, Gauss-Newton's method uses the descent direction:

$$\delta \mathbf{x}^{(k)} = -\left(\sum_{j=1}^{n} J_j(\mathbf{x}^{(k)})^{\top} J_j(\mathbf{x}^{(k)})\right)^{-1} \left(\sum_{j=1}^{n} J_j(\mathbf{x}^{(k)})^{\top} \mathbf{e}_j(\mathbf{x}^{(k)})\right)$$
$$= -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} (A_j \mathbf{x}^{(k)} + b_j)\right)$$
$$= -\mathbf{x}^{(k)} - \left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

If α^(k) = 1, in this problem, Gauss-Newton's method behaves exactly like Newton's method and coverges in one iteration!

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