

# ECE276A: Sensing & Estimation in Robotics

## Lecture 2: Unconstrained Optimization

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# Outline

Linear Algebra Review

Unconstrained Optimization

Gradient Descent

Newton's and Gauss-Newton's Methods

Example

# Field

- ▶ A **field** is a set  $\mathcal{F}$  with two binary operations,  $+$  :  $\mathcal{F} \times \mathcal{F} \mapsto \mathcal{F}$  (addition) and  $\cdot$  :  $\mathcal{F} \times \mathcal{F} \mapsto \mathcal{F}$  (multiplication), which satisfy the following axioms:
  - ▶ **Associativity**:  $a + (b + c) = (a + b) + c$  and  $a(bc) = (ab)c$ ,  $\forall a, b, c \in \mathcal{F}$
  - ▶ **Commutativity**:  $a + b = b + a$  and  $ab = ba$ ,  $\forall a, b \in \mathcal{F}$
  - ▶ **Identity**:  $\exists 1, 0 \in \mathcal{F}$  such that  $a + 0 = a$  and  $a1 = a$ ,  $\forall a \in \mathcal{F}$
  - ▶ **Inverse**:  $\forall a \in \mathcal{F}, \exists -a \in \mathcal{F}$  such that  $a + (-a) = 0$   
 $\forall a \in \mathcal{F} \setminus \{0\}, \exists a^{-1} \in \mathcal{F} \setminus \{0\}$  such that  $aa^{-1} = 1$
  - ▶ **Distributivity**:  $a(b + c) = (ab) + (ac)$ ,  $\forall a, b, c \in \mathcal{F}$
- ▶ **Examples**: real numbers  $\mathbb{R}$ , complex numbers  $\mathbb{C}$ , rational numbers  $\mathbb{Q}$

# Vector Space

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

## Basis and Dimension

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

## Inner Product and Norm

- ▶ An **inner product** on a vector space  $\mathcal{V}$  over a field  $\mathcal{F}$  is a function  $\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \mapsto \mathcal{F}$  such that for all  $a \in \mathcal{F}$  and all  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{V}$ :
  - ▶  $\langle a\mathbf{x}, \mathbf{y} \rangle = a\langle \mathbf{x}, \mathbf{y} \rangle$  (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)
  - ▶  $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$  (non-negativity)
  - ▶  $\langle \mathbf{x}, \mathbf{x} \rangle = 0$  iff  $\mathbf{x} = \mathbf{0}$  (definiteness)
- ▶ A **norm** on a vector space  $\mathcal{V}$  over a field  $\mathcal{F}$  is a function  $\| \cdot \| : \mathcal{V} \rightarrow \mathbb{R}$  such that for all  $a \in \mathcal{F}$  and all  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$ :
  - ▶  $\| a\mathbf{x} \| = |a| \| \mathbf{x} \|$  (absolute homogeneity)
  - ▶  $\| \mathbf{x} + \mathbf{y} \| \leq \| \mathbf{x} \| + \| \mathbf{y} \|$  (triangle inequality)
  - ▶  $\| \mathbf{x} \| \geq 0$  (non-negativity)
  - ▶  $\| \mathbf{x} \| = 0$  iff  $\mathbf{x} = \mathbf{0}$  (definiteness)

## Euclidean Vector Space

- ▶ A **Euclidean vector space**  $\mathbb{R}^d$  is a vector space with finite dimension  $d$  over the real numbers  $\mathbb{R}$
- ▶ A **Euclidean vector**  $\mathbf{x} \in \mathbb{R}^d$  is a collection of scalars  $x_i \in \mathbb{R}$  for  $i = 1, \dots, d$  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:  $\mathbf{x}^\top = [x_1 \ \cdots \ x_d]$
- ▶ 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  $\|\mathbf{x}\|_2 := \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} = \sqrt{\mathbf{x}^\top \mathbf{x}}$

## Matrices

- ▶ A real  $m \times n$  **matrix**  $A$  is a rectangular array of scalars  $A_{ij} \in \mathbb{R}$  for  $i = 1, \dots, m$  and  $j = 1, \dots, n$
- ▶ The set  $\mathbb{R}^{m \times n}$  of real  $m \times n$  matrices is a vector space
- ▶ The entries of the **transpose**  $A^T \in \mathbb{R}^{n \times m}$  of a matrix  $A \in \mathbb{R}^{m \times n}$  are  $A_{ij}^T = A_{ji}$ . The transpose satisfies:  $(AB)^T = B^T A^T$
- ▶ The **trace** of a matrix  $A \in \mathbb{R}^{n \times n}$  is the sum of its diagonal entries:

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

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

$$\langle X, Y \rangle = \text{tr}(X^T Y)$$

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



## Matrix Determinant and Inverse

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

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

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  $i^{\text{th}}$ -row and  $j^{\text{th}}$ -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:

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

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

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

## Eigenvalues and Eigenvectors

- ▶ 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  $\mathbf{q}$  is an **eigenvector** corresponding to the **eigenvalue**  $\lambda$ .

- ▶ The  $n$  eigenvalues of  $A \in \mathbb{R}^{n \times n}$  are the  $n$  roots of the **characteristic polynomial**  $p_A(s)$  of  $A$ :

$$p_A(s) := \det(sI - A)$$

- ▶ A real matrix can have complex eigenvalues and eigenvectors, which appear in conjugate pairs.
- ▶ Eigenvectors are not unique since for any  $c \in \mathbb{C} \setminus \{0\}$ ,  $c\mathbf{q}$  is an eigenvector corresponding to the same eigenvalue.

# Diagonalization

- ▶ Let  $\lambda$  be an eigenvalue of  $A \in \mathbb{R}^{n \times n}$
- ▶ Let  $p_A(s)$  be the characteristic polynomial of  $A$
- ▶ The **algebraic multiplicity** of  $\lambda$  is the number of times  $(s - \lambda)$  occurs as a factor of  $p(s)$
- ▶ The **geometric multiplicity** of  $\lambda$  is the dimension of its eigenspace  $\ker(A - \lambda I)$
- ▶ The geometric multiplicity of  $\lambda$  is less than or equal to its algebraic multiplicity
- ▶  $A$  is diagonalizable if and only the sum of its eigenspace dimensions equals  $n$
- ▶ If the eigenvalues of  $A$  are distinct, then  $A$  is diagonalizable

## Eigenvalue Decomposition

- ▶ **Eigen decomposition:** if  $A \in \mathbb{R}^{n \times n}$  is diagonalizable, then  $n$  linearly independent eigenvectors  $\mathbf{q}_i$  can be found:

$$A\mathbf{q}_i = \lambda_i\mathbf{q}_i, \quad i = 1, \dots, n$$

The eigen decomposition of  $A$  is obtained by stacking the  $n$  equations:

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

- ▶ **Jordan decomposition:**  $A \in \mathbb{R}^{n \times n}$  can be decomposed using an invertible matrix of generalized eigenvectors  $Q$  and an upper-triangular matrix  $J$ :

$$A = QJQ^{-1}$$

- ▶ **Jordan form of  $A$ :** an upper-triangular block-diagonal matrix:

$$J = \text{diag}(B(\lambda_1, m_1), \dots, B(\lambda_k, m_k))$$

where  $\lambda_1, \dots, \lambda_k$  are the eigenvalues of  $A$  and  $m_1 + \dots + m_k = n$  are their algebraic multiplicities.

$$B(\lambda, m) = \begin{bmatrix} \lambda & 1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \lambda & 1 \\ 0 & 0 & 0 & \lambda \end{bmatrix} \in \mathbb{R}^{m \times m}$$

## Singular Value Decomposition

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

$$A = U\Sigma V^T \quad \Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & \end{bmatrix} \in \mathbb{R}^{m \times n}$$

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

## Matrix Pseudo Inverse

- ▶ The **pseudo-inverse**  $A^\dagger \in \mathbb{R}^{n \times m}$  of  $A \in \mathbb{R}^{m \times n}$  can be obtained from its SVD  $A = U\Sigma V^T$ :

$$A^\dagger = V\Sigma^\dagger U^T \quad \Sigma^\dagger = \begin{bmatrix} 1/\sigma_1 & & & \\ & \ddots & & \\ & & 1/\sigma_r & \\ & & & \end{bmatrix} \in \mathbb{R}^{n \times m}$$

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

## 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  $A = U\Sigma V^T$  and rank  $r$
- ▶ The **column space** or **image** of  $A$  is  $im(A) \subseteq \mathbb{R}^m$  and is spanned by the  $r$  columns of  $U$  corresponding to non-zero singular values
- ▶ The **null space** or **kernel** of  $A$  is  $ker(A) \subseteq \mathbb{R}^n$  and is spanned by the  $n - r$  columns of  $V$  corresponding to zero singular values
- ▶ The **row space** or **co-image** of  $A$  is  $im(A^T) \subseteq \mathbb{R}^n$  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  $ker(A^T) \subseteq \mathbb{R}^m$  and is spanned by the  $m - r$  columns of  $U$  corresponding to zero singular values
- ▶ The **domain** of  $A$  is  $\mathbb{R}^n = ker(A) \oplus im(A^T)$
- ▶ The **co-domain** of  $A$  is  $\mathbb{R}^m = ker(A^T) \oplus im(A)$

## 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  $A = U\Sigma V^T$  and rank  $r$
- ▶ If  $\mathbf{b} \in im(A)$ , i.e.,  $\mathbf{b}^T \mathbf{v} = 0$  for all  $\mathbf{v} \in ker(A^T)$ , then  $A\mathbf{x} = \mathbf{b}$  has **one or infinitely many solutions**  $\mathbf{x} = A^\dagger \mathbf{b} + (I - A^\dagger A)\mathbf{y}$  for any  $\mathbf{y} \in \mathbb{R}^n$
- ▶ If  $\mathbf{b} \notin im(A)$ , then **no solution exists** and  $\mathbf{x} = A^\dagger \mathbf{b}$  is an approximate solution with minimum  $\|\mathbf{x}\|$  and  $\|A\mathbf{x} - \mathbf{b}\|$  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  $\mathbf{x}^\top A \mathbf{x}$  with  $A \in \mathbb{R}^{n \times n}$  and  $\mathbf{x} \in \mathbb{R}^n$  is called **quadratic form** and  $A$  can be assumed **symmetric**,  $A = A^\top$ , because:

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

- ▶ A symmetric matrix  $A \in \mathbb{R}^{n \times n}$  is **positive semidefinite** if  $\mathbf{x}^\top A \mathbf{x} \geq 0$  for all  $\mathbf{x} \in \mathbb{R}^n$ .
- ▶ 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.

## Matrix Derivatives (Numerator Layout)

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

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

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

$$\frac{dy}{d\mathbf{x}} = \underbrace{\begin{bmatrix} \frac{dy}{dx_1} & \cdots & \frac{dy}{dx_p} \end{bmatrix}}_{[\nabla_{\mathbf{x}}y]^T \text{ (gradient transpose)}} \in \mathbb{R}^{1 \times p} \quad \frac{d\mathbf{y}}{d\mathbf{x}} = \underbrace{\begin{bmatrix} \frac{dy_1}{dx_1} & \cdots & \frac{dy_1}{dx_p} \\ \vdots & \ddots & \vdots \\ \frac{dy_m}{dx_1} & \cdots & \frac{dy_m}{dx_p} \end{bmatrix}}_{\text{Jacobian}} \in \mathbb{R}^{m \times p}$$

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

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

## Matrix Derivative Examples

- ▶  $\frac{d}{dX_{ij}} X = \mathbf{e}_i \mathbf{e}_j^\top$
- ▶  $\frac{d}{dx} A\mathbf{x} = A$
- ▶  $\frac{d}{dx} \mathbf{u}^\top \mathbf{v} = \mathbf{u}^\top \frac{d\mathbf{v}}{dx} + \mathbf{v}^\top \frac{d\mathbf{u}}{dx}$  (product rule)
- ▶  $\frac{d}{dx} \mathbf{x}^\top A\mathbf{x} = \mathbf{x}^\top (A + A^\top)$
- ▶  $\frac{d}{dx} M^{-1}(x) = -M^{-1}(x) \frac{dM(x)}{dx} M^{-1}(x)$
- ▶  $\frac{d}{dX} \text{tr}(AX^{-1}B) = -X^{-1}BAX^{-1}$
- ▶  $\frac{d}{dX} \log \det X = X^{-1}$

## Matrix Derivative Examples

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

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

$$\blacktriangleright M(x)M^{-1}(x) = I \quad \Rightarrow \quad 0 = \left[ \frac{d}{dx} M(x) \right] M^{-1}(x) + M(x) \left[ \frac{d}{dx} M^{-1}(x) \right]$$

$$\begin{aligned} \blacktriangleright \frac{d}{dX_{ij}} \operatorname{tr}(\mathbf{A}\mathbf{X}^{-1}\mathbf{B}) &= \operatorname{tr}\left(\mathbf{A} \frac{d}{dX_{ij}} \mathbf{X}^{-1} \mathbf{B}\right) = -\operatorname{tr}(\mathbf{A}\mathbf{X}^{-1} \mathbf{e}_i \mathbf{e}_j^\top \mathbf{X}^{-1} \mathbf{B}) \\ &= -\mathbf{e}_j^\top \mathbf{X}^{-1} \mathbf{B} \mathbf{A} \mathbf{X}^{-1} \mathbf{e}_i = -\mathbf{e}_i^\top (\mathbf{X}^{-1} \mathbf{B} \mathbf{A} \mathbf{X}^{-1})^\top \mathbf{e}_j \end{aligned}$$

$$\begin{aligned} \blacktriangleright \frac{d}{dX_{ij}} \log \det X &= \frac{1}{\det(X)} \frac{d}{dX_{ij}} \sum_{k=1}^n X_{ik} \operatorname{cof}_{ik}(X) \\ &= \frac{1}{\det(X)} \operatorname{cof}_{ij}(X) = \frac{1}{\det(X)} \operatorname{adj}_{ji}(X) = \mathbf{e}_j^\top \mathbf{X}^{-1} \mathbf{e}_i \end{aligned}$$

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Example

# Unconstrained Optimization

- ▶ **Unconstrained optimization problem** over Euclidean vector space  $\mathbb{R}^d$ :

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

- ▶ 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 of  $\mathbf{x}_*$  (e.g., an open ball with small radius centered at  $\mathbf{x}_*$ ). The value  $f(\mathbf{x}_*)$  is called **local minimum**.
- ▶ The function  $f : \mathbb{R}^d \mapsto \mathbb{R}$  is **differentiable** at  $\mathbf{x} \in \mathbb{R}^d$  if its gradient exists:

$$\nabla f(\mathbf{x}) := \left[ \frac{\partial f(\mathbf{x})}{\partial x_1} \quad \dots \quad \frac{\partial f(\mathbf{x})}{\partial x_d} \right]^T \in \mathbb{R}^d$$

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

## Descent Direction

- ▶ Consider an unconstrained optimization problem:

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

### Descent Direction Theorem

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

# 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.

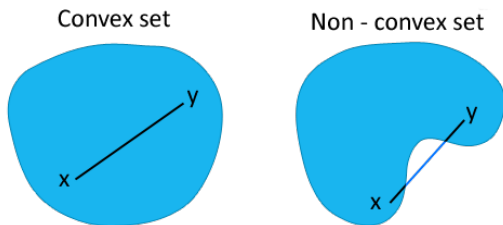
## Necessary and Sufficient Condition

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



## 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



- ▶ A function  $f : \mathcal{D} \mapsto \mathbb{R}$  with  $\mathcal{D} \subseteq \mathbb{R}^d$  is **convex** if:
  - ▶  $\mathcal{D}$  is a convex set
  - ▶  $f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1 - \lambda)f(\mathbf{y})$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{D}$ ,  $\lambda \in [0, 1]$
- ▶ **First-order convexity condition:** a differentiable  $f : \mathcal{D} \mapsto \mathbb{R}$  with convex  $\mathcal{D}$  is convex iff  $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{D}$
- ▶ **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 Optimization Methods

- ▶ A critical point of  $f$  can be obtained by solving  $\nabla f(\mathbf{x}) = 0$  but an explicit solution may be difficult to obtain
- ▶ **Descent method:** iterative method to obtain a solution of  $\nabla f(\mathbf{x}) = 0$
- ▶ Given initial guess  $\mathbf{x}_k$ , take step of size  $\alpha_k > 0$  along descent direction  $\delta\mathbf{x}_k$ :

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \delta\mathbf{x}_k$$

- ▶ Different descent methods differ in the way  $\delta\mathbf{x}_k$  and  $\alpha_k$  are chosen
- ▶  $\delta\mathbf{x}_k$  needs to be a descent direction:  $\nabla f(\mathbf{x}_k)^\top \delta\mathbf{x}_k < 0, \forall \mathbf{x}_k \neq \mathbf{x}_*$
- ▶  $\alpha_k$  needs to ensure sufficient decrease in  $f$  to guarantee convergence:
  - ▶ The best step size choice is  $\alpha_k \in \arg \min_{\alpha > 0} f(\mathbf{x}_k + \alpha \delta\mathbf{x}_k)$
  - ▶ In practice,  $\alpha_k$  is obtained via approximate **line search** methods

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## Gradient Descent (First-Order Method)

- ▶ **Idea:**  $-\nabla f(\mathbf{x}_k)$  points in the direction of steepest 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  $\alpha_k$  is  $\frac{1}{L}$ , where  $L > 0$  is the Lipschitz constant of  $\nabla f(\mathbf{x})$ :

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

### Gradient Descent Convergence

Suppose  $f$  is twice continuously differentiable with

$$ml \preceq \nabla^2 f(\mathbf{x}) \preceq Ll, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

The iterates  $\mathbf{x}_k$  of gradient descent with step size  $\alpha_k = \frac{1}{L}$  satisfy:

$$\|\nabla f(\mathbf{x}_k)\| \rightarrow 0 \quad \text{and} \quad \|\mathbf{x}_k - \mathbf{x}_*\| \rightarrow 0 \quad \text{as } k \rightarrow \infty.$$

## Proof: Gradient Descent Convergence

- ▶ By the Mean Value Theorem for some  $\mathbf{c}_k$  between  $\mathbf{x}_k$  and  $\mathbf{x}_{k+1}$ :

$$\nabla f(\mathbf{x}_{k+1}) = \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{c}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k) = \nabla f(\mathbf{x}_k) - \alpha_k \nabla^2 f(\mathbf{c}_k) \nabla f(\mathbf{x}_k)$$

- ▶ Let  $\lambda_i$  be the eigenvalues of  $\nabla^2 f(\mathbf{c}_k)$  so that:

$$0 \leq 1 - \alpha_k L \leq 1 - \alpha_k \lambda_i \leq 1 - \alpha_k m$$

- ▶ This is sufficient to show that  $\|\nabla f(\mathbf{x}_k)\| \rightarrow 0$  linearly:

$$\|\nabla f(\mathbf{x}_{k+1})\| \leq (1 - m/L) \|\nabla f(\mathbf{x}_k)\| \leq (1 - m/L)^{k+1} \|\nabla f(\mathbf{x}_0)\|$$

- ▶ By the Mean Value Theorem for some  $\tilde{\mathbf{c}}_k$  between  $\mathbf{x}_k$  and  $\mathbf{x}_*$ :

$$\mathbf{x}_{k+1} - \mathbf{x}_* = (\mathbf{x}_k - \mathbf{x}_*) - \alpha_k (\nabla f(\mathbf{x}_k) - \nabla f(\mathbf{x}_*)) = (\mathbf{x}_k - \mathbf{x}_*) - \alpha_k \nabla^2 f(\tilde{\mathbf{c}}_k) (\mathbf{x}_k - \mathbf{x}_*)$$

- ▶ Since  $mI \preceq \nabla^2 f(\tilde{\mathbf{c}}_k) \preceq LI$ :

$$\|\mathbf{x}_{k+1} - \mathbf{x}_*\| \leq (1 - m/L) \|\mathbf{x}_k - \mathbf{x}_*\| \leq (1 - m/L)^{k+1} \|\mathbf{x}_0 - \mathbf{x}_*\|$$

# Projected Gradient Descent

- ▶ **Constrained optimization problem** over a closed convex set  $\mathcal{C} \subseteq \mathbb{R}^n$ :

$$\min_{\mathbf{x} \in \mathcal{C}} f(\mathbf{x})$$

- ▶ **Constrained optimality condition**: for differentiable convex function  $f$ :

$$\mathbf{x}_* \in \arg \min_{\mathbf{x} \in \mathcal{C}} f(\mathbf{x}) \quad \Leftrightarrow \quad \langle \nabla f(\mathbf{x}_*), \mathbf{y} - \mathbf{x}_* \rangle \geq 0, \quad \forall \mathbf{y} \in \mathcal{C}$$

- ▶ **Euclidean projection onto  $\mathcal{C}$** :

$$\Pi_{\mathcal{C}}(\mathbf{x}) := \arg \min_{\mathbf{y} \in \mathcal{C}} \|\mathbf{y} - \mathbf{x}\|$$

- ▶ **Projected gradient descent**:

$$\mathbf{x}_{k+1} = \Pi_{\mathcal{C}}(\mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k)), \quad \alpha > 0$$

# Projected Gradient Descent

## Projected Gradient Descent Convergence

Suppose  $f$  is twice continuously differentiable with

$$ml \preceq \nabla^2 f(\mathbf{x}) \preceq Ll, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

The iterates  $\mathbf{x}_k$  of projected gradient descent with step size  $\alpha = \frac{1}{L}$  satisfy:

$$\|\mathbf{x}_{k+1} - \mathbf{x}_*\| \leq (1 - m/L)^{k+1} \|\mathbf{x}_0 - \mathbf{x}_*\|.$$

- ▶ The proof is based on:
  - ▶ Euclidean projection is non-expansive:

$$\|\Pi_C(\mathbf{x}) - \Pi_C(\mathbf{y})\| \leq \|\mathbf{x} - \mathbf{y}\|, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$$

- ▶ Constrained optimizers are fixed points of the projected gradient descent operator with  $\alpha > 0$ :

$$\mathbf{x}_* \in \arg \min_{\mathbf{x} \in C} f(\mathbf{x}) \quad \Leftrightarrow \quad \mathbf{x}_* = \Pi_C(\mathbf{x}_* - \alpha \nabla f(\mathbf{x}_*))$$

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## Newton's Method (Second-Order Method)

- ▶ Consider an unconstrained optimization problem:

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

- ▶ **Newton's method** iteratively approximates  $f$  by a quadratic function
- ▶ For a small change  $\delta \mathbf{x}$  to  $\mathbf{x}_k$ , we can approximate  $f$  using Taylor series:

$$\begin{aligned} f(\mathbf{x}_k + \delta \mathbf{x}) &\approx f(\mathbf{x}_k) + \underbrace{\left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}=\mathbf{x}_k} \right)}_{\text{gradient transpose}} \delta \mathbf{x} + \frac{1}{2} \delta \mathbf{x}^\top \underbrace{\left( \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} \Big|_{\mathbf{x}=\mathbf{x}_k} \right)}_{\text{Hessian}} \delta \mathbf{x} \\ &=: \underbrace{q(\delta \mathbf{x}, \mathbf{x}_k)}_{\text{quadratic function in } \delta \mathbf{x}} \end{aligned}$$

- ▶ The symmetric Hessian matrix  $\nabla^2 f(\mathbf{x}_k)$  needs to be positive-definite for this method to work



## Newton's Method (Second-Order Method)

- ▶ Find  $\delta \mathbf{x}$  that minimizes the quadratic approximation to  $f(\mathbf{x}_k + \delta \mathbf{x})$ :

$$\min_{\delta \mathbf{x} \in \mathbb{R}^d} q(\delta \mathbf{x}, \mathbf{x}_k)$$

- ▶ Since this is an unconstrained optimization problem,  $\delta \mathbf{x}$  can be determined by setting the derivative of  $q$  with respect to  $\delta \mathbf{x}$  to zero:

$$0 = \frac{\partial q(\delta \mathbf{x}, \mathbf{x}_k)}{\partial \delta \mathbf{x}} = \nabla f(\mathbf{x}_k)^\top + \delta \mathbf{x}^\top \nabla^2 f(\mathbf{x}_k)$$

- ▶ This is a linear system of equations in  $\delta \mathbf{x}$  and can be solved uniquely when the Hessian is invertible, i.e.,  $\nabla^2 f(\mathbf{x}_k) \succ 0$ :

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

- ▶ **Newton's method:**

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k [\nabla^2 f(\mathbf{x}_k)]^{-1} \nabla f(\mathbf{x}_k), \quad \alpha_k > 0$$

## Newton's Method (Second-Order Method)

- ▶ Like other descent methods, Newton's method converges to a local minimum
- ▶ **Damped Newton phase:** when the iterates are “far away” from the optimum, the function value is decreased sublinearly, i.e., the step sizes  $\alpha_k$  are small
- ▶ **Quadratic convergence phase:** when the iterates are “sufficiently close” to the optimum, full Newton steps are taken, i.e.,  $\alpha_k = 1$ , and the function value converges quadratically to the optimum
- ▶ A **disadvantage** of Newton's method is the need to form the Hessian  $\nabla^2 f(\mathbf{x}_k)$ , which can be numerically ill-conditioned or 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:

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

- ▶ Derivative and Hessian:

$$\text{Jacobian:} \quad \left. \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} = \mathbf{e}(\mathbf{x}_k)^\top \left( \left. \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} \right)$$

$$\begin{aligned} \text{Hessian:} \quad \left. \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} \right|_{\mathbf{x}=\mathbf{x}_k} &= \left( \left. \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} \right)^\top \left( \left. \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} \right) \\ &\quad + \sum_{i=1}^m e_i(\mathbf{x}_k) \left( \left. \frac{\partial^2 e_i(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} \right|_{\mathbf{x}=\mathbf{x}_k} \right) \end{aligned}$$

## Gauss-Newton's Method

- ▶ Near the minimum of  $f$ , the second term in the Hessian is small relative to the first. The Hessian can be approximated without second derivatives:

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

- ▶ Approximation of  $f(\mathbf{x}_k + \delta \mathbf{x})$ :

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

- ▶ Setting the gradient of this new quadratic approximation of  $f$  with respect to  $\delta \mathbf{x}$  to zero, leads to the system:

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

- ▶ **Gauss-Newton's method:**

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \delta \mathbf{x}, \quad \alpha_k > 0$$

## Gauss-Newton's Method (Alternative Derivation)

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

$$\mathbf{e}(\mathbf{x}_k + \delta\mathbf{x}) \approx \mathbf{e}(\mathbf{x}_k) + \left( \left. \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} \right) \delta\mathbf{x}$$

- ▶ Substituting into  $f$  leads to:

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

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

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

## Levenberg-Marquardt's Method

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

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

- ▶  $\lambda D$  compensates for the missing Hessian term  $\sum_{i=1}^m e_i(\mathbf{x}_k) \left( \frac{\partial^2 e_i(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^\top} \Big|_{\mathbf{x}=\mathbf{x}_k} \right)$
- ▶ When  $\lambda \geq 0$  is large, the descent direction  $\delta \mathbf{x}$  corresponds to a small step in the direction of steepest descent. This helps when the Hessian approximation is poor or poorly conditioned by providing a meaningful direction.



## Gauss-Newton's Method (Summary)

- ▶ An iterative optimization approach for the unconstrained problem:

$$\min_{\mathbf{x}} f(\mathbf{x}) := \frac{1}{2} \sum_j \mathbf{e}_j(\mathbf{x})^\top \mathbf{e}_j(\mathbf{x}) \quad \mathbf{e}_j(\mathbf{x}) \in \mathbb{R}^{m_j}, \mathbf{x} \in \mathbb{R}^n$$

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

- ▶ Obtain an updated estimate according to:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \delta \mathbf{x}, \quad \alpha_k > 0$$

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## 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  $\min_{\mathbf{x}} f(\mathbf{x})$  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  $\mathbf{x}_0 = \mathbf{0}$
- ▶ At iteration  $k$ , gradient descent uses the descent direction  $\delta\mathbf{x}_k = -\nabla f(\mathbf{x}_k)$
- ▶ Determine the Lipschitz constant of  $\nabla f(\mathbf{x})$ :

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

- ▶ Choose step size  $\alpha_k = \frac{1}{L}$  and iterate:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha_k \delta\mathbf{x}_k \\ &= \mathbf{x}_k - \frac{1}{L} \left( \sum_{j=1}^n A_j^\top A_j \right) \mathbf{x}_k - \frac{1}{L} \left( \sum_{j=1}^n A_j^\top b_j \right) \end{aligned}$$

## Newton's Method

- ▶ Start with an initial guess  $\mathbf{x}_0 = \mathbf{0}$
- ▶ At iteration  $k$ , Newton's method uses the descent direction:

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

- ▶ With  $\alpha_k = 1$ , Newton's method converges in one iteration:

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

## 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:

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

- ▶ With  $\alpha_k = 1$ , in this problem, Gauss-Newton's method behaves like Newton's method and converges in one iteration