



MSML610: Advanced Machine Learning

Linear Algebra

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References:

Linear algebra

- **Linear algebra**
 - Vector and vector spaces
 - Affine spaces
 - Vectors and matrices
 - Linear functions
 - Connections between Machine Learning and Linear Algebra

Vector and vector spaces

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Field: definition

A field $\mathbb{F} = (X, +, *)$ is a set X with two binary operations $+$ and $*$, satisfying the following 6 axioms:

1. Closed with respect to $+$ and $*$:

$$a, b \in X \implies a + b \in X$$

$$a, b \in X \implies a * b \in X$$

2. Commutativity of $+$ and $*$:

$$a + b = b + a$$

$$a * b = b * a$$

3. Associativity of $+$ and $*$:

$$a + (b + c) = (a + b) + c = a + b + c$$

$$a * (b * c) = (a * b) * c = a * b * c$$

4. Distributivity of multiplication over addition:

$$a * (b + c) = a * b + a * c$$

5. Existence of $+$ and $*$ identity elements, 0 and 1:

$$a + 0 = a$$

Field: examples

- Examples
 - The set of $\mathbb{R}, \mathbb{C}, \text{GF}(2)$
 - The set of rational numbers \mathbb{Q} , i.e., numbers that can be written as fraction $\frac{a}{b}$ with $a, b \in \mathbb{Z}$ and $b \neq 0$
- Non-examples
 - The set of positive integers $\mathbb{N} = 1, 2, 3, \dots$ is not a field
 - The set of integers $\mathbb{Z} = \dots, -2, -1, 0, 1, 2, \dots$ is not a field

Vector space: definition

- A “vector space \mathcal{V} over a field \mathbb{F} ” is a triple $(\mathcal{V}, \mathbb{F}, +, \cdot)$ where:
 - \mathcal{V} is a set of vectors
 - \mathbb{F} is a field of scalars
 - $+$ is a sum operation between vectors
 - \cdot is a scalar multiplication
- A vector space needs to satisfy the following 2 properties:
 1. Closed with respect to scalar multiplication: if $\underline{x} \in \mathcal{V}$, then $\alpha \cdot \underline{x} \in \mathcal{V}$
 2. Closed with respect to vector addition: if $\underline{x}, \underline{y} \in \mathcal{V}$, then $\underline{x} + \underline{y} \in \mathcal{V}$

Linear combination of vectors

- The vector

$$\alpha_1 \underline{\mathbf{v}}_1 + \alpha_2 \underline{\mathbf{v}}_2 + \dots + \alpha_n \underline{\mathbf{v}}_n$$

is a linear combination of vectors $\underline{\mathbf{v}}_1, \dots, \underline{\mathbf{v}}_n$ with coefficients $\alpha_1, \dots, \alpha_n$

- A linear combination can be written in matrix form:

$$\underline{\underline{\mathbf{V}}} \cdot \underline{\underline{\alpha}} \text{ or } \underline{\underline{\alpha}}^T \cdot \underline{\underline{\mathbf{V}}}^T$$

where $\underline{\underline{\mathbf{V}}} = (\underline{\mathbf{v}}_1 | \dots | \underline{\mathbf{v}}_n)$

Span of vectors

- The span of n m -dimensional vectors is the set of all linear combinations of the n vectors:

$$\text{Span}(\underline{\mathbf{v}}_1, \dots, \underline{\mathbf{v}}_n) = \{\underline{\mathbf{V}} \cdot \underline{\boldsymbol{\alpha}} \text{ with } \underline{\boldsymbol{\alpha}} \in \mathbb{F}^n\} = \{\underline{\mathbf{v}} \in \mathbb{F}^m : \underline{\mathbf{v}} = \sum_{i=1}^n \alpha_i \underline{\mathbf{v}}_i\}$$

- E.g., the span of vectors is a vector space

Null space of a matrix

- Null space of the columns of a matrix $\underline{\underline{\mathbf{A}}}$ is defined as the set:

$$\text{Null}(\underline{\underline{\mathbf{A}}}) = \{\underline{\underline{\mathbf{v}}} : \underline{\underline{\mathbf{A}}} \cdot \underline{\underline{\mathbf{v}}} = \underline{\underline{\mathbf{0}}}\}$$

- In words, all the vectors that are coefficients of linear combinations of columns of $\underline{\underline{\mathbf{A}}}$ yielding the zero vector
- Null space is a vector space

Homogeneous linear system associated with null space

- From the definition of matrix-vector multiplication the vector $\underline{\mathbf{v}}$ is in $\text{Null}(\underline{\underline{\mathbf{A}}}) \iff \underline{\mathbf{v}}$ is a solution of the homogeneous linear system involving the columns of $\underline{\underline{\mathbf{A}}}$:

$$\underline{\mathbf{a}}_1^T \cdot \underline{\mathbf{v}} = 0$$

$$\underline{\mathbf{a}}_2^T \cdot \underline{\mathbf{v}} = 0$$

...

$$\underline{\mathbf{a}}_m^T \cdot \underline{\mathbf{v}} = 0$$

- Note that the notation is a bit confusing since we mean the transpose of the columns $\underline{\mathbf{a}}_i$ of $\underline{\underline{\mathbf{A}}}$ and not the rows of $\underline{\underline{\mathbf{A}}}$

Dot product on a vector space: definition

- Given a field of scalars \mathbb{F} and a vector space \mathcal{V} over \mathbb{F} , an inner product is a mapping:

$$\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{F}$$

that satisfies the 3 axioms:

1. Conjugate symmetry (almost commutativity):

$$\langle \underline{x}, \underline{y} \rangle = \overline{\langle \underline{y}, \underline{x} \rangle}$$

2. Linearity in the first argument:

$$\langle a\underline{x}, \underline{y} \rangle = a\langle \underline{x}, \underline{y} \rangle$$

$$\langle \underline{x} + \underline{y}, \underline{z} \rangle = \langle \underline{x}, \underline{z} \rangle + \langle \underline{y}, \underline{z} \rangle$$

3. Positive definitiveness:

$$\langle \underline{x}, \underline{x} \rangle \geq 0$$

$$\langle \underline{x}, \underline{x} \rangle = 0 \implies \underline{x} = \underline{0}$$

Vector inner product

- Aka “dot product”, “scalar product”
- Given $\underline{\mathbf{x}}, \underline{\mathbf{y}} \in \mathbb{F}^n$ (i.e., same number of components and also same “label” for each element), the inner product of $\underline{\mathbf{x}}$ and $\underline{\mathbf{y}}$ is defined as:

$$\langle \underline{\mathbf{x}}, \underline{\mathbf{y}} \rangle = \underline{\mathbf{x}}^T \cdot \underline{\mathbf{y}} = \sum_{i=1}^n x_i y_i \in \mathbb{F}$$

- $\underline{\mathbf{x}}^T \cdot \underline{\mathbf{y}}$ is read “x dotted y” or “x transposed y”

Affine spaces

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Affine space: definition

- If \underline{c} is a vector and \mathcal{V} is a vector space then

$$\mathcal{A} = \underline{c} + \mathcal{V} = \{\underline{c} + \underline{v} : \underline{v} \in \mathcal{V}\}$$

is called an affine space

- An affine space is a vector space translated by a point represented by a vector
 - E.g., a plane or a line that do not contain the origin

Affine space: example of plane passing through 3 points

- Given 3 not collinear vectors: \underline{u}_1 , \underline{u}_2 , and \underline{u}_3 , the plane containing the endpoints of the 3 vectors can be represented as $\mathcal{A} = \underline{u}_1 + \mathcal{V}$ where $\mathcal{V} = \text{Span}(\underline{u}_2 - \underline{u}_1, \underline{u}_3 - \underline{u}_1)$
- **Note:** the span of the 3 vectors has dimension 3, but an affine space with dimension 2

Affine combination: definition

- An affine combination is a linear combination of vectors where the sum of the (positive or negative) coefficients is 1:

$$\alpha_1 \underline{\mathbf{u}}_1 + \dots + \alpha_n \underline{\mathbf{u}}_n \text{ where } \sum_i \alpha_i = 1$$

- In matrix form: $\underline{\mathbf{U}} \cdot \underline{\boldsymbol{\alpha}}$ where $\underline{\mathbf{1}}^T \underline{\boldsymbol{\alpha}} = 1$

Affine hull of vectors

- Given vectors $\underline{u}_1, \dots, \underline{u}_n$, the set of all affine combinations is the affine hull:

$$\mathcal{A} = \left\{ \underline{v} = \sum_i^n \alpha_i \underline{u}_i : \sum_i \alpha_i = 1 \right\} = \left\{ \underline{v} = \underline{\underline{U}} \underline{\alpha} : \underline{\mathbf{1}}^T \underline{\alpha} = 1 \right\}$$

- The affine hull includes each point because if $\underline{\alpha}$ has a single 1 in position i and all others 0, we get \underline{u}_i

Affine hull of vectors is an affine space

- We can write the affine hull of $\underline{u}_1, \dots, \underline{u}_n$ as an affine space:

$$\underline{u}_i + \text{Span}(\underline{u}_1 - \underline{u}_i, \dots, \underline{u}_n - \underline{u}_i)$$

- Thus an affine space is an affine hull and vice versa
- This is the dual of “the span of vectors is a vector space”

The solution set of non-homogeneous linear system is empty or affine space

- Consider the solution of a system of non-homogeneous linear equations

$$\{\underline{x} : \underline{a}_1^T \underline{x} = \beta_1, \dots, \underline{a}_m^T \underline{x} = \beta_m\} \text{ or in matrix form } \underline{\underline{A}} \cdot \underline{x} = \underline{\beta}$$

- The solution set is either empty or an affine space
- There are two cases: either the non-homogeneous system has solution, or not
- Consider the case where the system of equations has no solutions (e.g., it is contradictory, e.g., $x = 1, x = 2$), then the solution set is empty
- Consider the case where there is a solution
- Each linear system $\underline{\underline{A}}\underline{x} = \underline{\beta}$ has an associated homogeneous linear system $\underline{\underline{A}}\underline{x} = \underline{0}$
- If \underline{u}_1 is a solution of the non-homogeneous system (i.e., $\underline{\underline{A}}\underline{u}_1 = \underline{\beta}$), then any other solution \underline{u}_2 is a solution (i.e., $\underline{\underline{A}}\underline{u}_2 = \underline{\beta}$) $\iff \underline{u}_2 - \underline{u}_1$ is in the vector space which is the solution of the homogeneous linear system (i.e., $\underline{\underline{A}}(\underline{u}_1 - \underline{u}_2) = \underline{0}$)

Vector space vs affine space: summary

- Linear combination vs affine combination
- Span of vectors vs affine hull of vectors
 - Span (affine hull) is the set of all linear (affine) combinations
- Vector space vs affine space

Vectors and matrices

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Matrices and Matrix Operations

- A matrix $\underline{\underline{\mathbf{A}}} \in \mathbb{F}^{m \times n}$ is a two dimensional array with dimensions $m \times n$ of elements from a field \mathbb{F}
- Matrix notation
 - $\underline{\underline{\mathbf{A}}} \in \mathbb{R}^{m \times n}$ has m rows and n columns
 - $\underline{\underline{A}}_{ij}$ is the element on i -th row and j -th column

$$\underline{\underline{\mathbf{A}}} = \begin{pmatrix} A_{1,1} & \dots & A_{1,n} \\ \dots & A_{i,j} & \dots \\ A_{m,1} & \dots & A_{m,n} \end{pmatrix}$$

- The convention is first rows and then columns (i.e., y-x instead of the more usual x-y) for both elements and dimensions of a matrix
- Notation for rows and columns in a matrix
 - j -th column is $\underline{\underline{\mathbf{a}}}_j$ or $\underline{\underline{\mathbf{a}}}_{:,j}$ (using numpy notation)
 - i -th row is $\underline{\underline{\mathbf{a}}}_i^T$ or $\underline{\underline{\mathbf{a}}}_{i,:}$
 - Fixing a coordinate (e.g., row) one gets the orthogonal indices (e.g., column)

Linear functions

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Linear functions over vector spaces: definition

- Consider two vector spaces \mathcal{V} and \mathcal{W} over the same field \mathbb{F}
- A linear function $f : \mathcal{V} \rightarrow \mathcal{W}$ satisfies two properties:
 1. $f(\alpha \underline{\mathbf{v}}) = \alpha f(\underline{\mathbf{v}})$
 2. $f(\underline{\mathbf{u}} + \underline{\mathbf{v}}) = f(\underline{\mathbf{u}}) + f(\underline{\mathbf{v}})$
- Linear functions “push linear combination through”:

$$f(\alpha_1 \underline{\mathbf{v}}_1 + \dots + \alpha_n \underline{\mathbf{v}}_n) = \alpha_1 f(\underline{\mathbf{v}}_1) + \dots + \alpha_n f(\underline{\mathbf{v}}_n)$$

- This is equivalent to the 2 properties of linear functions

From matrix to linear function

- Given a matrix $\underline{\underline{\mathbf{A}}} \in \mathbb{F}^{n \times m}$ we can define the function:

$$f(\underline{\mathbf{x}}) = \underline{\underline{\mathbf{A}}} \cdot \underline{\mathbf{x}}$$

- The function $f()$ maps m -vectors into n -vectors
 - The domain is \mathbb{F}^m for the matrix-vector product to be defined
 - The co-domain is \mathbb{F}^n
 - MEM: the inputs are from the top and the outputs from the side
- $f(\underline{\mathbf{x}})$ is a linear function because of the properties of matrix-vector product

From linear function to matrix

- Consider a linear function $f : \mathbb{F}^m \rightarrow \mathbb{F}^n$
- We want to find a matrix $\underline{\underline{\mathbf{A}}}$ such that $f(\underline{\mathbf{x}}) = \underline{\underline{\mathbf{A}}} \cdot \underline{\mathbf{x}}$
- ***Solution***
- We know that $\underline{\underline{\mathbf{A}}} \in \mathbb{F}^{n \times m}$ from matrix-vector product definition, but what are the elements of $\underline{\underline{\mathbf{A}}}$?
- Note that if we compute $\underline{\underline{\mathbf{A}}} \cdot \underline{\mathbf{e}}_i$, where $\mathbf{e}_i = (0, \dots, 0, 1, \dots, 0)$ is the i -th standard generator, we obtain $\underline{\mathbf{a}}_i$ (i.e., the i -th column of $\underline{\underline{\mathbf{A}}}$)
- Thus $\underline{\underline{\mathbf{A}}}$ is the matrix with columns equal to the standard generators transformed by $f()$

Linear functions: examples and non-examples

- The identity function corresponds to the identity matrix
- A diagonal matrix corresponds to a transformation scaling each coordinate independently
- Rotation and scaling are linear transformations
- Translation is not a linear function, since it does not satisfy either of the two linearity properties

A linear function maps zero vector to zero vector

- It can be proved that a linear function $f : \mathcal{V} \rightarrow \mathcal{W}$ maps the zero vector of \mathcal{V} to the zero vector of \mathcal{W}

Kernel of a function

- The kernel of a (linear) function f is the set of vectors that are transformed by f into the $\underline{\mathbf{0}}$ vector

$$\text{Ker}(f) = \{\underline{\mathbf{v}} : f(\underline{\mathbf{v}}) = \underline{\mathbf{0}}\}$$

Kernel of a linear function and null space of matrix

- If f is written in terms of a matrix as $f(\underline{x}) = \underline{\underline{A}} \cdot \underline{x}$ then:

$$\text{Ker}(f) = \text{Null}(\underline{\underline{A}})$$

- The kernel of a linear function is the null space of the columns of the associated matrix $\underline{\underline{A}}$

Domain

- Consider a function $f : \mathcal{V} \rightarrow \mathcal{W}$
- \mathcal{V} “domain”: the set of all values where the function is defined

Image of domain

- Consider a function $f : \mathcal{V} \rightarrow \mathcal{W}$
- $f(\mathcal{V})$ “image of domain”: the set of all values that the function can assume

Codomain

- \mathcal{W} “co-domain”: the set where the function assumes its value (e.g., \mathbb{R}^2)
- Note that often it is not easy to describe $f(\mathcal{V})$ in a compact way so we use $\mathcal{W} \supseteq f(\mathcal{V})$

One-to-one function: definition

- Aka injective
- Consider a function $f : \mathcal{V} \rightarrow \mathcal{W}$
- A function is one-to-one \iff two different elements $v_1 \neq v_2 \in \mathcal{V}$ have different images $f(v_1) \neq f(v_2)$
- Equivalent definition using contrapositive
 - One-to-one function \iff two elements v_1 and v_2 have the same image $f(v_1) = f(v_2)$, then they are equal $v_1 = v_2$
- Equivalent definition in terms of set cardinality
 - One-to-one function $\iff |f(\mathcal{V})| = |\mathcal{V}|$, i.e., the image of the domain has the same number of elements as the domain

Onto function

- Aka surjective
- Consider a function $f : \mathcal{V} \rightarrow \mathcal{W}$
- A function is onto \iff for any element of its co-domain $w \in \mathcal{W}$, there exists an element of the domain $v \in \mathcal{V}$ that is transformed into it, i.e., $f(v) = w$
- Equivalent definition in terms of set cardinality
 - Onto function $\iff f(\mathcal{V}) = \mathcal{W}$, i.e., the image of the domain is equal to the co-domain
 - Note that any function can be made surjective by restricting \mathcal{W} to $f(\mathcal{V})$

Invertible function

- A function $f : \mathcal{V} \rightarrow \mathcal{W}$ is invertible \iff it is both one-to-one (injective) and onto (surjective)
- Equivalently: $\forall w \in \mathcal{W} \exists ! v \in \mathcal{V} : f(v) = w$
- Equivalent definition in terms of set cardinality
 - Invertible function $\iff |\mathcal{V}| = |\mathcal{W}|$, i.e., the co-domain and the domain have the same number of elements

Inverse of a function

- The inverse of f is $f^{-1} : \mathcal{W} \rightarrow \mathcal{V}$ and $f \circ f^{-1}$ is the identity function

One-to-one lemma for linear functions

- A linear function is one-to-one \iff its kernel is the trivial vector space, i.e., $\text{Ker}(f) = \{\underline{\mathbf{0}}\}$
- Equivalently the associated matrix $\underline{\underline{\mathbf{A}}}$ has $\text{Null}(\underline{\underline{\mathbf{A}}}) = \{\underline{\mathbf{0}}\}$

Matrix-matrix multiplication and linear function composition

- We have seen that there is a correspondence between linear functions and matrices
- What does composition of linear functions correspond to?
- Consider two matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ and the two associated functions:
 $f(\underline{y}) = \underline{\underline{A}} \cdot \underline{y}$ and $g(\underline{x}) = \underline{\underline{B}} \cdot \underline{x}$
- The composed function is $h(\underline{x}) = (f \circ g)(\underline{x}) = f(g(\underline{x}))$
- It can be shown that: $h(\underline{x}) = \underline{\underline{A}} \cdot \underline{\underline{B}} \cdot \underline{x}$

Matrix inverse

- Using the definition of inverse functions, two square matrices $\underline{\underline{\mathbf{A}}}$ and $\underline{\underline{\mathbf{B}}}$ are inverses $\iff \underline{\underline{\mathbf{A}}} \cdot \underline{\underline{\mathbf{B}}} = \underline{\underline{\mathbf{I}}}$
- We indicate the (unique) inverse of $\underline{\underline{\mathbf{A}}}$ with $\underline{\underline{\mathbf{A}}}^{-1}$

Invertible matrix and solution of matrix-vector equation

- Given an invertible (square) matrix $\underline{\underline{\mathbf{A}}}$, then $f(\underline{\mathbf{x}}) = \underline{\underline{\mathbf{A}}} \cdot \underline{\mathbf{x}}$ is an invertible function, i.e., $f()$ is one-to-one and onto
- Thus the matrix-vector equation $\underline{\underline{\mathbf{A}}} \cdot \underline{\mathbf{x}} = \underline{\mathbf{b}}$ has one and only one solution $\underline{\mathbf{x}}$ for any $\underline{\mathbf{b}}$, i.e., $\underline{\underline{\mathbf{A}}}^{-1} \underline{\mathbf{b}}$

Invertibility of matrix-matrix product

- If $\underline{\underline{\mathbf{A}}}$ and $\underline{\underline{\mathbf{B}}}$ are invertible and can be multiplied, then $\underline{\underline{\mathbf{A}}} \cdot \underline{\underline{\mathbf{B}}}$ is invertible

Systems of Linear Equations

- Represented as $Ax = b$
- Solutions using Gaussian elimination
- Conditions for existence and uniqueness

Rank of a Matrix

- Number of linearly independent rows or columns
- Rank-nullity theorem: $\text{rank}(A) + \text{nullity}(A) = n$
- Implications for solution spaces

Inverse of a Matrix

- Matrix A is invertible if $AA^{-1} = I$
- Not all matrices are invertible (singular matrices)
- Importance for solving linear systems and optimization

Determinants

- Scalar value summarizing matrix properties
- Zero determinant implies matrix is singular
- Used in volume interpretation and invertibility

Orthogonality and Orthonormal Bases

- Two vectors are orthogonal if $x^T y = 0$
- Orthonormal set: orthogonal unit vectors
- Used in projections, decomposition, and optimization

Projections and Least Squares

- Projection of b onto column space of A : $\hat{b} = A(A^T A)^{-1} A^T b$
- Basis for linear regression
- Solves inconsistent systems approximately

Eigenvalues and Eigenvectors

- For $Ax = \lambda x$, x is an eigenvector and λ an eigenvalue
- Capture invariant directions of transformations
- Used in PCA, spectral clustering, and stability analysis

Diagonalization

- Expressing matrix as $A = PDP^{-1}$ where D is diagonal
- Simplifies powers and exponentials of matrices
- Requires linearly independent eigenvectors

Symmetric Matrices

- $A = A^T$
- All eigenvalues are real
- Basis of many ML methods (e.g., covariance matrices, kernels)

Positive Definite and Semidefinite Matrices

- $x^T A x > 0$ for all $x \neq 0$: positive definite
- Ensures convexity in optimization
- Common in loss functions and kernels

Singular Value Decomposition (SVD)

- Factorization: $A = U\Sigma V^T$
- Generalizes eigen-decomposition to all matrices
- Used in PCA, matrix compression, and pseudoinverse

Principal Component Analysis (PCA)

- Dimensionality reduction via eigen-decomposition of covariance matrix
- Projects data onto directions of maximum variance
- Computed using SVD in practice

Matrix Norms

- Measures of matrix size: Frobenius, spectral, etc.
- Important for measuring errors and convergence
- Used in regularization and optimization

Vector Norms

- L^p norms (e.g., L^1 , L^2)
- Measure magnitude of vectors
- Used in loss functions and sparsity enforcement

Trace of a Matrix

- Sum of diagonal entries: $\text{Tr}(A)$
- Invariant under cyclic permutations: $\text{Tr}(ABC) = \text{Tr}(CAB)$
- Appears in matrix derivatives and expectation identities

Kronecker and Hadamard Products

- Kronecker: tensor product of matrices
- Hadamard: element-wise multiplication
- Important in multi-dimensional ML models and tensor operations

Matrix Calculus

- Derivatives of scalar functions w.r.t. vectors/matrices
- Gradient and Hessian computation
- Crucial for backpropagation and optimization algorithms

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