COMP 7180 Quantitative Methods for Data Analytics and Artificial Intelligence

Lecture 2 – Linear Independence, Rank, and Orthogonality

Open Questions

AB ≠ BA (the commutative "law" is usually broken)

- 1. Are there any relations between AB and BA?
 - 2. If so, what are they?

Open Questions

- Solve Ax = b
- Suppose A is a square matrix and A is invertible.

$$Ax = b$$
 (multiply both sides by A^{-1})
 $A^{-1}Ax = A^{-1}b$ ($A^{-1}A = I$)
 $x = A^{-1}b$

Questions (We will answer them in the following lectures):

- 1. Which square matrices are invertible?
- 2. What if A is square matrix but not invertible?
- 3. What if A is not a square matrix?

Transpose Matrix

The transpose of A is denoted by A^T . Its columns are taken directly from the rows of A — the i-th row of A becomes the i-th column of A^T :

Transpose If
$$A = \begin{bmatrix} 2 & 1 & 4 \\ 0 & 0 & 3 \end{bmatrix}$$
 then $A^{T} = \begin{bmatrix} 2 & 0 \\ 1 & 0 \\ 4 & 3 \end{bmatrix}$

If A is an m by n matrix, then A^T is n by m. The final effect is to flip the matrix across its main diagonal, and the entry:

Entries of
$$A^{\mathrm{T}}$$
 $(A^{\mathrm{T}})_{ij} = A_{ji}$.

Properties of Transpose

- $(A+B)^T = A^T + B^T$
- The transpose of AB is $(AB)^T = B^TA^T$

Start from
$$AB = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 3 & 3 \\ 2 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 3 & 3 \\ 5 & 5 & 5 \end{bmatrix}$$

Transpose to $B^{T}A^{T} = \begin{bmatrix} 3 & 2 \\ 3 & 2 \\ 3 & 2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 5 \\ 3 & 5 \\ 3 & 5 \end{bmatrix}$.

Properties of Transpose

- The transpose of A^{-1} is $(A^{-1})^T = (A^T)^{-1}$
- Why?
- To establish the formula for $(A^{-1})^T$, start from $AA^{-1} = I$. Take transpose, we have $(AA^{-1})^T = I^T = I$.
- From the previous slides, we know $(AA^{-1})^T = (A^{-1})^T A^T$.
- So we have $(A^{-1})^T A^T = I$. This indicates that $(A^{-1})^T$ is the inverse of A^T , i.e., $(A^{-1})^T = (A^T)^{-1}$.

Inverse of
$$A^{T}$$
 = Transpose of A^{-1}

Symmetric Matrix

- A symmetric matrix is a matrix that equals its own transpose: $A^T = A$.
 - Each entry on one side of the diagonal equals its "mirror image" on the other side: $a_{ii} = a_{ii}$.

Symmetric matrices
$$A = \begin{bmatrix} 1 & 2 \\ 2 & 8 \end{bmatrix}$$
 and $D = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix}$

- Property: R^TR and RR^T are symmetric matrices.
- Why:

$$(R^TR)^T = R^T(R^T)^T = R^TR$$
 (since $(R^T)^T = R$)
 $(RR^T)^T = (R^T)^TR^T = RR^T$

Small Exercise

If A is not a zero matrix, is A² = 0 possible? is A^TA = 0 possible?

• Solution: $A^2 = 0$ is possible.

• On the other hand, $A^TA = 0$ is not possible, which can be proved by exploring its diagonal.

More Advanced Content

- Linear Independence, Basis, Rank, and Dimension
- Orthogonality

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Rank r:

- Physical meaning: the amount of useful and non-redundant information in the data (matrix)
- Formal definition: The number of independent rows/columns in the matrix A.
- $-m=n=r \Rightarrow \text{invertible}$
- Definition of linear independence and dependence:
 - Suppose $c_1v_1 + \cdots + c_kv_k = 0$ only happens when $c_1 = \cdots = c_k = 0$. Then the vectors v_1, \dots, v_k are <u>linearly independent</u>.
 - If any c's are(is) nonzero, the v's are <u>linearly dependent</u>. One vector is a combination of the others.

$$A = \begin{bmatrix} 1 & 3 & 3 & 2 \\ 2 & 6 & 9 & 5 \\ -1 & -3 & 3 & 0 \end{bmatrix}$$

 Example 1. The columns of the above matrix are linearly dependent, since the second column is three times the first.

<u>Example 2</u>. The columns of the following triangular matrix are linearly independent.

No zeros on the diagonal
$$A = \begin{bmatrix} 3 & 4 & 2 \\ 0 & 1 & 5 \\ 0 & 0 & 2 \end{bmatrix}$$

Solve
$$Ac = 0$$

$$c_1 \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 4 \\ 1 \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} 2 \\ 5 \\ 2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

 c_1 , c_2 , c_3 are all forced to be zero.

- A set of n vectors in \mathbf{R}^m must be linearly dependent if n > m.
- Example 3. The three columns of the following matrix cannot be independent

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 1 & 3 & 2 \end{bmatrix}$$

In-Class Exercise 1

If w1, w2, w3 are independent vectors, let

$$v1 = w2 - w3,$$

 $v2 = w1 - w3,$
 $v3 = w1 - w2.$

- Are v1, v2, and v3 independent?
- Solution: No, because v1 v2 + v3 = 0.

In-Class Exercise 2

If w1, w2, w3 are independent vectors, let

$$v1 = w2 + w3,$$

 $v2 = w1 + w3,$
 $v3 = w1 + w2.$

- Are v1, v2, and v3 independent?
- Solution: Yes. Assume that c1*v1+c2*v2+c3*v3 = 0. Then we have c1*(w2+w3)+c2*(w1+w3)+c3*(w1+w2) = 0. Then we have (c2+c3)*w1 + (c1+c3)*w2 + (c1+c2)*w3 = 0. We know that w1, w2, w3 are independent, so we have c2+c3=0, c1+c3=0, and c1+c2=0, which gives us c1=c2=c3=0. So v1, v2, and v3 are independent.

Vector Spaces

- Most important spaces:
 - 1. R¹: Line (One-dimensional space)
 - 2. \mathbb{R}^2 : Represented by usual x-y plane (Two-dimensional space)
 - 3. \mathbb{R}^3 : Represented by usual x-y-z space (Three-dimensional space)
- A real vector space is a set of vectors together with rules for vector addition and multiplication by real numbers
 - Linear combinations stay in the vector space
 - If we add any vectors x and y in the vector space, x+y is in the vector space.
 - If we multiply any vector x in the vector space by any scalar c, cx is in the vector space.

Spanning a Vector Space

- If a vector space \mathbf{V} consists of all linear combinations of w_1, \dots, w_l , then these vectors **span the space**. Every vector v in \mathbf{V} is some combination of the w's:
- Every v comes from w's: $v = c_1 w_1 + \cdots + c_l w_l$ for some coefficients c_i .

Basis for a Vector Space

- The crucial idea of a basis:
 - A basis for V is a sequence of vectors having two properties at once:
 - 1. The vectors are linearly independent (not too many vectors).
 - 2. They span the space **V** (not too few vectors).
- A vector space has <u>infinitely many different bases</u>.
- Whenever a square matrix is invertible, its columns are independent—and they are a basis for \mathbb{R}^n .

Dimension of a Vector Space

- The number of basis vectors is a property of the space itself:
 - Any two bases for a vector space V contain the same number of vectors.
 - This number, which is shared by all bases and expresses the number of "degrees of freedom" of the space, is the <u>dimension</u> of V.

Dimension of a Vector Space

- In a subspace of dimension k, no set of more than k vectors can be independent, and no set of less than k vectors can span the space.
 - Any linearly independent set in V can be extended to a basis, by adding more vectors
 if necessary. (A basis is a <u>maximal independent set</u>. It cannot be made larger
 without losing independence.)
 - Any spanning set in V can be reduced to a basis, by discarding vectors if necessary.
 (A basis is also a <u>minimal spanning set</u>. It cannot be made smaller and still span the space.)

In-Class Exercise 3

Suppose v_1, v_2, \dots, v_6 are six vectors in \mathbb{R}^4 .

- (a) Those vectors (do)(do not) (might not) span \mathbb{R}^4 .
- (b) Those vectors (are) (are not) (might be) linearly independent.
- (c) Any four of those vectors (are)(are not) (might be) a basis for \mathbb{R}^4 .

More Advanced Content

- Linear Independence, Basis, Rank, and Dimension
- Orthogonality

Orthogonality and Independence

Useful fact: If nonzero vectors $v_1, ..., v_k$ are mutually orthogonal, then those vectors are linearly independent.

Why?

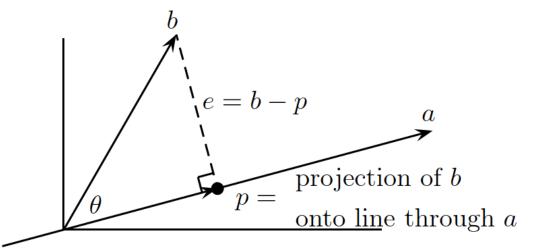
- Suppose $c_1v_1 + \cdots + c_kv_k = 0$.
- Orthogonality of the v's leaves only one term:

$$v_1^{\mathrm{T}}(c_1v_1+\cdots+c_kv_k)=c_1v_1^{\mathrm{T}}v_1=0.$$

- The vectors are nonzero, so $v_1^T v_1 \neq 0$ and therefore $c_1 = 0$.
- The same is true of every c_i . So the only combination of the v's producing zero has all $c_i = 0$: **independence**!

Projections

- Suppose we want to find the distance from a point b to the line in the direction of the vector a.
 - The dotted line connecting b to p is orthogonal/perpendicular to a.
- Given a plane (or any vector space
 S) instead of a line, again the problem is to find the point p on that space that is closest to b.
 - This point p is the projection of b onto the vector space.



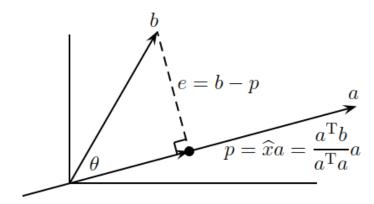
Projection onto a Line

- Find the projection point p:
 - All we need is the geometrical fact that the line from b to the closest point $p = \hat{a} = \hat{x}a$ is orthogonal to the vector a:

$$(b-\widehat{a})\perp a$$
, or $a^{\mathrm{T}}(b-\widehat{a})=0$, or $\widehat{x}=\frac{a^{\mathrm{T}}b}{a^{\mathrm{T}}a}$.

- The projection of the vector b onto the line in the direction of a is $p = \hat{x}a$:

Projection onto a line
$$p = \widehat{x}a = \frac{a^{\mathrm{T}}b}{a^{\mathrm{T}}a}a.$$



Projection Matrix of Rank 1

- The projection of b onto the line through a lies at $p = a(a^Tb/a^Ta)$.
- Projection onto a line is carried out by a <u>projection matrix</u> P. P is the matrix that multiplies b and produces p:

$$p = a \frac{a^{\mathrm{T}} b}{a^{\mathrm{T}} a}$$
 so the projection matrix is $P = \frac{a a^{\mathrm{T}}}{a^{\mathrm{T}} a}$.

Example

• The matrix that projects onto the line through $a = (1,1,1)^T$ is:

$$P = \frac{aa^{\mathrm{T}}}{a^{\mathrm{T}}a} = \frac{1}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}.$$

- *P* is a symmetric matrix.
- Its square is itself: $P^2 = P$.
 - ➤ Why?
 - > What does it mean?

Projections and Least Squares

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• Ax = b either has solution(s) or not. More equations 2x = b_1 than unknowns— 3x = b_2 no solution? 4x = b_3.
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- In spite of their unsolvability, <u>inconsistent equations arise all</u> the time in practice. They have to be solved!
 - Rather than expecting no error in some equations and large errors in the others, it is much better to choose the x that minimizes an average error E in the m equations.

Projections and Least Squares

The most convenient "average" comes from the sum of squares:

Squared error
$$E^2 = (2x - b_1)^2 + (3x - b_2)^2 + (4x - b_3)^2$$
. $2x = b_1$
 $3x = b_2$

- If there is an exact solution, the minimum error is E = 0. $4x = b_3$.
- In the more likely case that b is not proportional to a, the graph of E^2 will be a parabola (抛物線). The minimum error is at the lowest point, where the derivative is zero:

$$\frac{dE^2}{dx} = 2[(2x - b_1)2 + (3x - b_2)3 + (4x - b_3)4] = 0.$$

– Solving for x, the least-squares solution of this model system ax = b is denoted by \hat{x} :

Leastsquares solution
$$\widetilde{x} = \frac{2b_1 + 3b_2 + 4b_3}{2^2 + 3^2 + 4^2} = \frac{a^{\text{T}}b}{a^{\text{T}}a}.$$

Projections and Least Squares

The **general case** is the same, We "solve" ax = b by minimizing:

$$E^2 = ||ax - b||^2 = (a_1x - b_1)^2 + \dots + (a_mx - b_m)^2.$$

• The derivative of E^2 is zero at the point \hat{x} , if:

$$(a_1\hat{x} - b_1)a_1 + \dots + (a_m\hat{x} - b_m)a_m = 0.$$

• We are minimizing the distance from b to the line through a, and calculus gives the same answer, $\hat{x} = (a_1b_1 + \dots + a_mb_m)/(a_1^2 + \dots + a_m^2)$, that geometry did earlier:

The least-squares solution to a problem ax = b in one unknown is $\hat{x} = \frac{a^T b}{a^T a}$.

• The error vector e connecting b to p must be perpendicular to a:

Orthogonality of
$$a$$
 and e $a^{T}(b-\widehat{x}a) = a^{T}b - \frac{a^{T}b}{a^{T}a}a^{T}a = 0.$

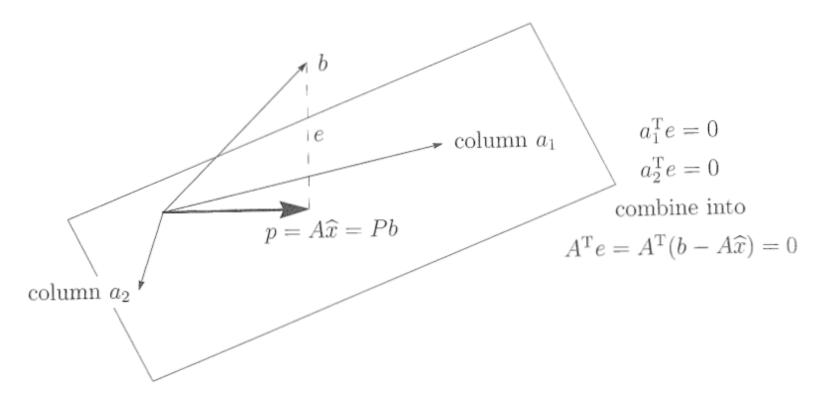
Least Squares Problems with Several Variables

- Now, projecting b onto a <u>vector space</u> rather than just onto a line. This problem arises from Ax = b when A is an m by n matrix.
 - The number m of equations is still larger than the number n of unknowns, so it must be expected that Ax = b will be inconsistent. **Probably, there will not exist a choice of** x **that perfectly fits the data** b.
- Again, the problem is to choose \hat{x} so as to minimize the error, and again this minimization will be done in the least-squares sense:
 - The error is E = ||Ax b||.
 - Searching for the least-squares solution \hat{x} , which minimizes E, is the same as locating the point $p = A\hat{x}$ that is closer to b than any other point in the column space.

Least Squares Problems with Several Variables

– We find \hat{x} and the projection $p = A\hat{x}$ as follows:

$$A^{\mathrm{T}}(b-A\widehat{x}) = 0$$
 or $A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}b$.



Normal Equations

- The equations $A^T A \hat{x} = A^T b$ are known in statistics as the **normal equations**.
 - When Ax = b is inconsistent, its least-squares solution minimizes $||Ax b||^2$:

Normal equations
$$A^{T}A\widehat{x} = A^{T}b$$
.

- A^TA is invertible exactly when the columns of A are linearly independent! Then:

Best estimate
$$\widehat{x}$$
 $\widehat{x} = (A^{T}A)^{-1}A^{T}b$.

– The projection of b onto the column space is the nearest point $A\hat{x}$:

Projection
$$p = A\widehat{x} = A(A^{T}A)^{-1}A^{T}b.$$

Projection Matrices

The closest point to b is $p = A(A^TA)^{-1}A^Tb$. The matrix that gives p is a **projection matrix**, denoted by P:

Projection matrix
$$P = A(A^{T}A)^{-1}A^{T}$$
.

Properties of Projection Matrices

- The projection matrix $P = A(A^TA)^{-1}A^T$ has two basic properties:
 - 1. It equals its square: $P^2 = P$.
 - 2. It equals its transpose: $P^T = P$.

– Why?

1. If we start with any b, then Pb lies in the subspace we are projecting onto. When we project again nothing is changed. P(Pb) is still Pb. Two or three or fifty projections give the same point p as the first projection:

$$P^2 = A(A^TA)^{-1}A^TA(A^TA)^{-1}A^T = A(A^TA)^{-1}A^T = P.$$

2. Multiply the transposes in reverse order, and use symmetry of $(A^TA)^{-1}$, to come back to P:

$$P^{T} = (A^{T})^{T} ((A^{T}A)^{-1})^{T} A^{T} = A(A^{T}A)^{-1} A^{T} = P.$$

Least-Squares Fitting of Data

- Suppose we do a series of experiments, and expect the output b to be a linear function of the input t.
- We look for a **straight line** b = C + Dt.
- How to compute C and D?

$$C + Dt_1 = b_1$$

$$C + Dt_2 = b_2$$

$$\vdots$$

$$C + Dt_m = b_m.$$

$$\begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}, \quad \text{or} \quad Ax = b.$$

• The best solution is (\hat{C}, \widehat{D}) that minimizes the squared error E^2 :

Minimize
$$E^2 = ||b - Ax||^2 = (b_1 - C - Dt_1)^2 + \dots + (b_m - C - Dt_m)^2$$
.

Example

• Supposing three measurements b_1 , b_2 , b_3 are marked:

$$b = 1$$
 at $t = -1$, $b = 1$ at $t = 1$, $b = 3$ at $t = 2$.

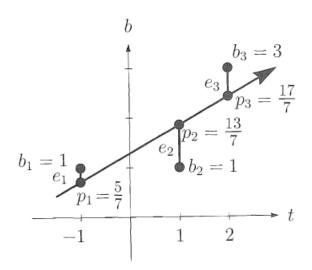
The first step is to write the equations:

$$Ax = b$$
 is $C - D = 1$ or $\begin{bmatrix} 1 & -1 \\ 1 & 1 \\ C + 2D = 3 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}$.

– They are solved by least squares:

$$A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}b$$
 is $\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{bmatrix} \widehat{C} \\ \widehat{D} \end{bmatrix} = \begin{bmatrix} 5 \\ 6 \end{bmatrix}$.

- The best solution is $\hat{C} = \frac{9}{7}$, $\widehat{D} = \frac{4}{7}$ and the best line is $\frac{9}{7} + \frac{4}{7}t$.



Orthonormal Basis

- In an <u>orthogonal basis</u>, every vector is perpendicular to every other vector.
- Divide each vector by its length, to make it a unit vector. That changes an orthogonal basis into an <u>orthonormal basis</u> of q's.
 - The vectors q_1, \dots, q_n are <u>orthonormal</u> if:

$$q_i^{\mathrm{T}}q_j = \begin{cases} 0 & \text{whenever } i \neq j, \\ 1 & \text{whenever } i = j, \end{cases}$$
 giving the orthogonality; giving the normalization.

A matrix with orthonormal columns will be called Q.

Standard Orthonormal Basis

- The most important example of Q is the <u>standard basis</u>:
 - For the x-y plane, the best-known axes $e_1 = (1,0)$ and $e_2 = (0,1)$.
 - In n dimensions the standard basis e_1, \dots, e_n again consists of the columns of Q = I:

Standard basis
$$e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \cdots, e_n = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}.$$

Orthogonal Matrices

• If Q has orthonormal columns, then $Q^TQ = I$:

• An orthogonal matrix is a square matrix with orthonormal columns. Its transpose is the inverse $Q^T = Q^{-1}$.

References and Acknowledgement

Strang G. Linear algebra and its applications[J]. 2000.

The End