COMP 7180 Quantitative Methods for Data Analytics and Artificial Intelligence

Lecture 2 – Linear Independence, Rank, and Orthogonality

What is Linear Algebra

- Linear algebra is the study of vectors, matrices, and linear functions/equations.
- Vectors (columns of numbers) and matrices (2D arrays of numbers) are the language of data.
- Linear algebra is a branch of mathematics, but the truth of it is that linear algebra is the mathematics of data.

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

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.

Small Exercise

• If A is not a zero matrix, is $A^2 = 0$ possible? is $A^TA = 0$ possible?

Outline of Today's 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.

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

 <u>Example 1.</u> 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?

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?

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

If $v_1, ..., v_m$ and $w_1, ..., w_n$ are both bases for the same vector space, then m = n. The number of vectors is the same.

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 .

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- Orthogonality

Orthogonality and Independence

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

Subspaces

- Definition: A <u>subspace</u> of a vector space is a nonempty subset that satisfies the requirements for a vector space: <u>Linear combinations stay in the subspace</u>.
 - I. If we add any vectors x and y in the subspace, x + y is in the subspace.
 - II. If we multiply any vector x in the subspace by any scalar c, cx is in the subspace.
- Notice: The zero vector will belong to every subspace.
- The smallest subspace Z contains only one vector, the zero vector.
- The largest subspace is the whole of the original space.

Orthogonal Subspaces

- The orthogonality of two subspaces:
 - Two subspaces V and W of the same space \mathbb{R}^n are orthogonal if every vector v in V is orthogonal to every vector w in W: $v^Tw = 0$ for all v and w.
 - Example:
 - Suppose V is the plane spanned by $v_1 = (1,0,0)$ and $v_2 = (0,1,0)$.
 - If **W** is the line spanned by w = (0,0,1), then w is orthogonal to both v's. The line **W** will be orthogonal to the whole plane **V**.

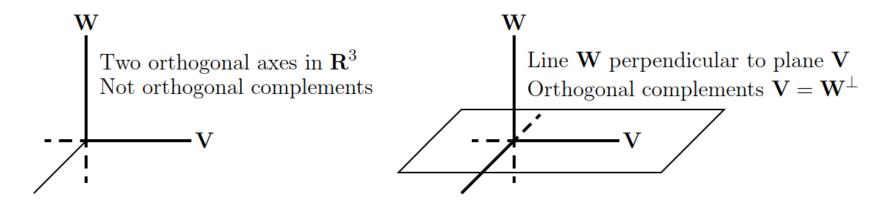
Orthogonal Complement

Definition:

– Given a subspace V of \mathbb{R}^n , the space of <u>all</u> vectors orthogonal to V is called the <u>orthogonal complement</u> of V. It is denoted by $V^{\perp} = V$ perp. ".

Splitting \mathbb{R}^n into Orthogonal Parts

- Orthogonal complements in R³:
 - The dimensions of V and W are right, and the whole space R³ is being decomposed into two perpendicular parts.



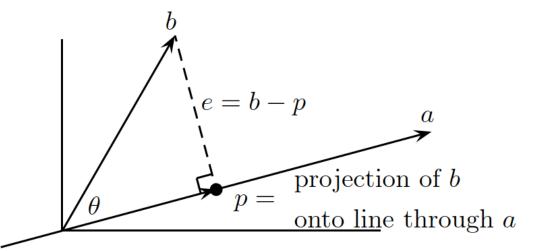
- Splitting \mathbb{R}^n into orthogonal parts will split every vector into x = v + w.
 - The vector v is the projection onto the subspace V.
 - The orthogonal component w is the projection of x onto \mathbf{W} .

Example

- Assume the whole space is R²
- If V is the subspace spanned by [1,0], then W is the subspace spanned by [0,1].
- Splitting \mathbb{R}^2 into orthogonal parts will split every vector into x = v + w. For example, x = [2,3] = [2,0] + [0,3]
 - v = [2,0] is the projection onto the subspace V.
 - The orthogonal component w = [0,3] is the projection of x onto **W**.

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 perpendicular to a.
- Given a plane (or any subspace S) instead of a line, again the problem is to find the point p on that subspace that is closest to b.
 - This point p is the projection of b onto the subspace.



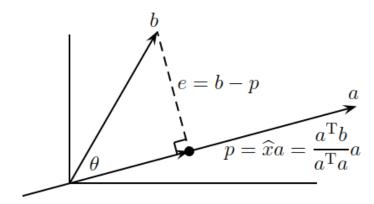
Projection onto a Line

- 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
$$p = \hat{x}a = \frac{a^{T}b}{a^{T}a}a.$$



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) 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: $P^2 = P$.
 - ➤ Can you prove that?
 - > 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 $a^{T}(b-\widehat{x}a) = a^{T}b - \frac{a^{T}b}{a^{T}a}a^{T}a = 0.$

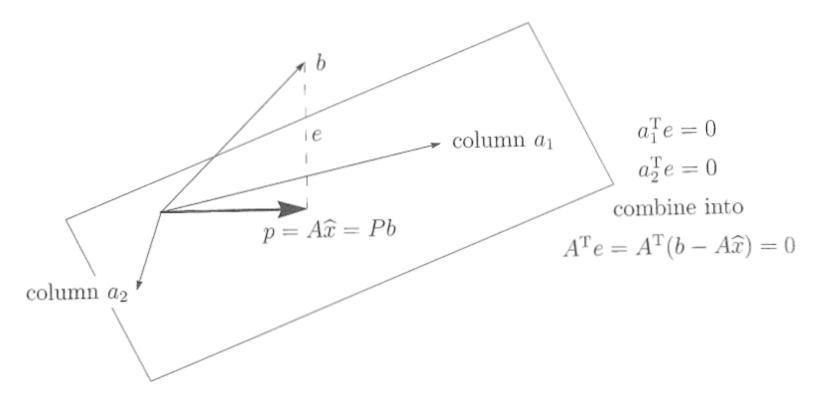
Least Squares Problems with Several Variables

- Now, projecting b onto a <u>subspace</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
$$p = A\widehat{x} = A(A^{T}A)^{-1}A^{T}b.$$

The Cross-Product Matrix A^TA

• The matrix A^TA is certainly **symmetric**.

$$- (A^T A)^T = A^T A^{TT} = A^T A$$

- $Ax = 0 \Rightarrow A^T Ax = 0$?
- $A^T A x = 0 \Rightarrow A x = 0$?

• A has independent columns $== A^T A$ is invertible.

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

- I - P is also a projection matrix! It projects b onto the orthogonal complement, and the projection is b - Pb.

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: $P^T = P$.

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. For example:

The cost of producing t books is nearly linear, b = C + Dt, with editing and typesetting in C and then printing and binding in D. C is the set-up cost and D is the cost for each additional book.

Least-Squares Fitting of Data

How to compute C and D?

$$C + Dt_1 = b_1$$

$$C + Dt_2 = b_2$$

$$\vdots$$

$$C + Dt_m = b_m.$$

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

- This is an <u>overdetermined</u> system, with m equations and only 2 unknowns.
 - If there is <u>no experimental error</u>, then two measurements of b will determine the line b = C + Dt.
 - If <u>errors are presenting</u>, it will have no solution.
- 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 $t = 2$.

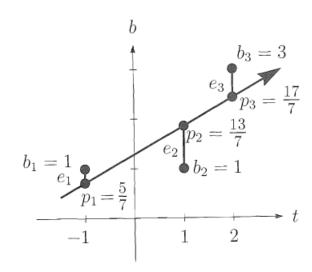
The first step is to write the equations:

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

– 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 $Q^T = Q^{-1}$.

Example

$$Q = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

$$Q^{T} = Q^{-1} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix}$$

- Q rotates every vector through the angle θ , and Q^T rotates it back through $-\theta$.
- The columns of Q and Q^T are <u>orthonormal</u> because $\sin^2 \theta + \cos^2 \theta = 1$.
- They are orthonormal matrices.

Properties of Orthogonal Matrix

Multiplication by any Q preserves lengths, because $(Qx)^T(Qx) = x^TQ^TQx = x^Tx$.

Lengths unchanged ||Qx|| = ||x|| for every vector x.

It also preserves inner products and angles, since $(Qx)^T(Qy) = x^TQ^TQy = x^Ty$.

Coefficients of the Basis Vectors

If we have an orthonormal basis, then any vector is a combination of the basis vectors. The problem is to find the coefficients of the basis vectors:

Write b as a combination
$$b = x_1q_1 + x_2q_2 + \cdots + x_nq_n$$
.

- 1 The method:
 - \triangleright Compute x_1 : Multiply both sides of the equation by q_1^T , we are left with:

$$q_1^{\mathrm{T}}b = x_1q_1^{\mathrm{T}}q_1.$$
 $q_1^{\mathrm{T}}q_1 = 1$ $x_1 = q_1^{\mathrm{T}}b.$

- >Similarly, the second coefficient is $x_2 = q_2^T b$.
- ▶ Each piece of b has a simple formula, and recombining the pieces gives back b:

Every vector b is equal to
$$(q_1^Tb)q_1 + (q_2^Tb)q_2 + \cdots + (q_n^Tb)q_n$$
.

Rectangular Matrices with Orthogonal Columns

- When the columns are orthonormal, the "cross-product matrix" A^TA becomes $Q^TQ = I$.
- We emphasize that those projections do not reconstruct b. In the square case m = n, they did. In the rectangular case m > n, they don't.
 - They give the projection p and not the original vector b and the q's are no longer a basis.
- The projection matrix is usually $A(A^TA)^{-1}A^T$, and here it simplifies to:

$$P = Q(Q^{\mathrm{T}}Q)^{-1}Q^{\mathrm{T}}$$
 or $P = QQ^{\mathrm{T}}$.

- Notice that Q^TQ is the n by n identity matrix, but QQ^T is an m by m projection P.

The End