

Lecture 3

Euclidean Vector Spaces and Projections

The defining condition of a real vector space $V \subset R^n$ is closure under linear transformations, i.e., $\alpha y + \gamma z \in V$ whenever $y, z \in V$ and $\alpha, \beta \in R$. Often we use the Euclidean norm $\|y\| = (y'y)^{1/2}$. Then, $(R^n, \|\cdot\|)$ is \mathcal{E}^n and \mathcal{E}^n is a normed vector space. Also, $(R^n, \langle \cdot, \cdot \rangle)$ is a Hilbert space (complete inner product space), where $\langle a, b \rangle = a'b$. A subset of a vector space that is a vector space in its own right is called a *linear subspace*.

Recall that the required properties of a norm are: for $a, b \in V$,

- (i) $\|a\| = 0$ iff $a = 0$
- (ii) $\|a + b\| \leq \|a\| + \|b\|$, and
- (iii) $\|\alpha a\| = |\alpha| \|a\|$ for $\alpha \in R$.

Also, the required properties of an inner product are

- (i) $\langle a, b \rangle = \langle b, a \rangle$,
- (ii) $\langle \alpha_1 a + \alpha_2 b, c \rangle = \alpha_1 \langle a, c \rangle + \alpha_2 \langle b, c \rangle$ for $\alpha_1, \alpha_2 \in R$, and
- (iii) $\langle a, a \rangle = \|a\|^2$.

Note that a normed vector space is complete if every absolutely summable sequence is summable. That is, if $\sum_{i=1}^{\infty} \|v_j\| < \infty$, then there exists a $v \in V$ such that $\|v - \sum_{i=1}^m v_j\| \rightarrow 0$ as $m \rightarrow \infty$.

Basis of a Vector Space

A set of vectors v_1, \dots, v_m is said to *span* a vector space $V \subset R^n$, if each $v \in V$ can be written as

$$v = \sum_{i=1}^m \alpha_i v_i \text{ for } \alpha_i \in R.$$

The smallest number of vectors that spans V is called the *dimension* of V . We will only consider finite dimensional vector spaces. Vectors v_1, \dots, v_m are linearly independent if $\sum_{i=1}^m \alpha_i v_i = 0 \Rightarrow \alpha_i = 0 \forall i \leq m$, where $\alpha_i \in R$. The largest number of linearly independent vectors is the dimension of V . (This is an equivalent definition of dimension.) A *basis* of a vector space V is any set of linearly independent vectors that spans V . From any basis we can always construct an *orthonormal basis*, i.e., a basis $\{v_i : i \leq \dim(V)\}$ whose vectors are of length one and are orthogonal:

$$v_i' v_i = 1, \quad v_i' v_j = 0, \quad i \neq j.$$

This can be proved using the Gram–Schmidt procedure. By definition, any $v \in V$ can be written in terms of an orthonormal basis v_1, \dots, v_p (where $p = \dim V$), because by definition v_1, \dots, v_p spans V , i.e., $v = \sum_{i=1}^p \alpha_i v_i$ for some $\alpha_i \in R \forall i \leq p$.

Furthermore, if $L \subset V$ is a linear subspace with orthonormal basis $\alpha_1, \dots, \alpha_q$, then we can find additional vectors $\alpha_{q+1}, \dots, \alpha_p$ such that $\alpha_1, \dots, \alpha_p$ span V and $\alpha_1, \dots, \alpha_p$ are orthonormal.

Proof: Consider different vectors until you obtain a collection that includes $\alpha_1, \dots, \alpha_q$ and that spans V . The number of vectors in the collection can be reduced to p linearly independent vectors

including $\alpha_1, \dots, \alpha_q$. Start with $\alpha_1, \dots, \alpha_q$ and use the Gram–Schmidt procedure to obtain the remaining $p - q$ orthonormal vectors.

The *orthogonal complement* of a linear subspace $L \subset V$ is defined by

$$L^\perp = \{z \in V : z' \ell = 0, \forall \ell \in L\}.$$

It is straightforward to see that L^\perp also is a linear subspace.

Theorem 1 (Vector Decomposition Theorem): Let V be a Hilbert space and let L be a linear subspace of V . Every element y of V can be written as the sum of two vectors y_1 and y_2 where $y_1 \in L$ and $y_2 \in L^\perp$. That is,

$$y = y_1 + y_2.$$

Proof: Let v_1, \dots, v_p be an orthonormal basis of L . Let $y_1 = \sum_{i=1}^p (y'v_i)v_i$. Let $y_2 = y - y_1$. Clearly, $y_1 \in L$. Also, for $j = 1, \dots, p$,

$$v'_j y_2 = v'_j (y - y_1) = v'_j y - v'_j \sum_{i=1}^p (y'v_i)v_i = v'_j y - v'_j v_j y' y = 0.$$

Hence, y_2 is orthogonal to $v_j, \forall j = 1, \dots, p$ and $y_2 \in L^\perp$. \square

An alternative way of expressing the above result is to say that $V = L \oplus L^\perp$. That is, V is the direct sum of L and L^\perp .

Let $y \in V$, a vector space. Let L be a linear subspace of V . An element of L is called a *projection* of y on L and is denoted $P_L y$, if

$$\|y - P_L y\| = \inf_{\ell \in L} \|y - \ell\|.$$

Theorem 2 (Projection Theorem): (a) $P_L y$ exists, is unique, and is a linear function of y . (b) $P_L y \in L$ is the projection of y on L iff $y - P_L y \perp L$. (That is, if we write $y = y_1 + y_2$ for $y_1 \in L, y_2 \in L^\perp$, then $y_1 = P_L y$.)

Proof: (a) By the proof that $V = L \oplus L^\perp$, we can write $y = y_1 + y_2$, where $y_1 \in L, y_2 \in L^\perp$, and $y_1 = \sum_{i=1}^p y'v_i v_i$. We want to show that $y_1 = P_L y$. If true, then $P_L y$ exists and is a linear function of y . Consider any $\ell \in L$. We have

$$\begin{aligned} \|y - \ell\|^2 &= \|y - y_1 + y_1 - \ell\|^2 \\ &= \|y - y_1\|^2 + \|y_1 - \ell\|^2 + 2(y - y_1)'(y_1 - \ell) \\ &= \|y - y_1\|^2 + \|y_1 - \ell\|^2 \\ &\geq \|y - y_1\|^2 \end{aligned}$$

with strict inequality unless $\|y_1 - \ell\| = 0$, i.e., unless $\ell = y_1$. (The inner product term is zero because $y - y_1 \in L^\perp$ and $y_1 - \ell \in L$.) Hence, y_1 is a projection of y on L and it is unique.

(b) If $P_L y$ is the projection of y on L , then by part (a) $P_L y = y_1$ and $y - P_L y = y_2 \in L^\perp$. Conversely, suppose $P_L y$ is some element of L for which $y - P_L y \in L^\perp$, then $y_1 + y_2 - P_L y \in L^\perp, y_1 - P_L y \in L^\perp, y_1 - P_L y \in L$ (since $y_1 \in L$ and $P_L y \in L$), and, hence, $y_1 - P_L y = 0$. That is, $P_L y$ is the projection of y on L . \square

We know that a projection is a linear map from V to L , so we may ask: How can such a linear map be characterized? Answer: It can be characterized in a simple way in terms of what it does to vectors in L and in L^\perp .

Theorem 3: The linear map $G : V \rightarrow L$ is the projection map onto L iff $Gy = y \ \forall y \in L$, and $Gy = 0 \ \forall y \in L^\perp$.

Proof: (a) Suppose G is the projection map from V to L . Then, if we consider $y \in L$, we find that y minimizes $\|y - \ell\|$ over $\ell \in L$ and so $Gy = y$. If $y \in L^\perp$, then $\|y - \ell\|^2 = \|y\|^2 + \|\ell\|^2$. The latter is minimized over $\ell \in L$ by $\ell = 0$, so Gy must equal 0.

(b) Conversely, suppose G is a linear map for which $Gy = y \ \forall y \in L$ and $Gy = 0 \ \forall y \in L^\perp$. Let y be any vector in V . By the vector decomposition theorem, we can write $y = y_1 + y_2$, where $y_1 \in L$ and $y_2 \in L^\perp$. In consequence, $Gy = Gy_1 + Gy_2 = y_1$. Note that $y - y_1 = y_2 \perp L$. So, by the projection theorem, $y_1 = P_L y$. That is, Gy is the projection of y on L . \square

Matrices as Linear Maps

An $n \times k$ matrix is just a linear transformation from \mathcal{E}^k to \mathcal{E}^n :

$$X(\alpha_1 y_1 + \alpha_2 y_2) = \alpha_1 Xy_1 + \alpha_2 Xy_2 \quad \forall y_1, y_2 \in \mathcal{E}^k, \forall \alpha_1, \alpha_2 \in R.$$

The *range* of the function (or linear map) X is $R(X) = \{x \in R^n : x = Xb \text{ for some } b \in R^k\}$. Alternatively, the range is called the *column space* of X , because $R(X)$ consists of all linear combinations of the columns of X .

Note that $R(X)$ is a vector space. It is a linear subspace of \mathcal{E}^n . This holds because

$$\begin{aligned} x_1, x_2 \in R(X) &\Rightarrow x_1 = Xb_1, \quad x_2 = Xb_2 \\ &\Rightarrow \alpha x_1 + \beta x_2 = X(\alpha b_1 + \beta b_2) \in R(X) \text{ since } \alpha b_1 + \beta b_2 \in R^k. \end{aligned}$$

Another linear subspace associated with X is a linear subspace of R^k called the *null space* of X . By definition, the null space of X is

$$N(X) = \{b \in R^k : Xb = 0\}.$$

Note that $N(X)$ is a linear subspace, because

$$\begin{aligned} b_1, b_2 \in N(X) &\Rightarrow X(\alpha b_1 + \beta b_2) = \alpha Xb_1 + \beta Xb_2 = 0 \\ &\Rightarrow \alpha b_1 + \beta b_2 \in N(X). \end{aligned}$$

The null space of X contains all vectors that are orthogonal or perpendicular to all rows of X .

The range space and null space of X are related as follows: $N(X) = R(X')^\perp$, where \perp denotes orthogonal complement. This holds because $b \perp R(X') \Leftrightarrow Xb = 0 \Leftrightarrow b \in N(X)$. This result implies that $R^k = R(X') \oplus N(X)$.

As an example, suppose

$$X = \begin{bmatrix} 1 & 1 \\ -2 & -2 \end{bmatrix}.$$

Then,

$$N(X) = \{y \in R^2 : Xy = 0\} = \{y : (1, 1)y = 0\} = \{y : y_1 = -y_2\}.$$

In addition, we have

$$\begin{aligned} X' &= \begin{bmatrix} 1 & -2 \\ 1 & -2 \end{bmatrix} \text{ and } R(X') = \{y : y = X'b \text{ for some } b \in R^2\} \\ &= \{y : y_1 = y_2\}. \end{aligned}$$

Thus, in this example, $N(X) = R(X')^\perp$.

Projection Maps

A projection map (like any linear map) can be represented as a matrix. What does such a matrix look like?

Theorem 4: For the Euclidean vector space $V \subset R^n$, a linear map $G : V \rightarrow V$ is a projection map (onto its range $R(G)$) iff $G' = G$ and $G^2 = G$. That is, iff G is symmetric and idempotent.

Proof: (a) Suppose G is a projection map. Let x, y be any vectors in V . Write $x = x_1 + x_2$ and $y = y_1 + y_2$, where $x_1, y_1 \in L$, $x_2, y_2 \in L^\perp$, and $L = R(G)$. Note that $x_1 = Gx$ and $y_1 = Gy$. Now,

$$\begin{aligned} x'G'y &= (Gx)'(y_1 + y_2) = (Gx)'y_1 && \text{because } Gx \in L, y_2 \in L^\perp \\ &= (x - x_2)'y_1 \\ &= x'y_1 && \text{because } x_2'y_1 = 0 \\ &= x'Gy. \end{aligned}$$

So, $G = G'$.

Also, $G^2y = G(Gy) = Gy$ because $Gy \in L$ and by the theorem above $Gx = x \forall x \in L$.

(b) Suppose $G^2 = G$ and $G = G'$. Let g be in $R(G)$. That is, $g = Gv$ for some $v \in V$. We need to show that $(y - Gy)'g = 0$. Then, the projection theorem implies that Gy is the projection of y on $R(G)$. But,

$$\begin{aligned} (y - Gy)'g &= (y - Gy)'Gv = [G(y - Gy)]'v && \text{by symmetry of } G \\ &= (Gy - Gy)'v && \text{by idempotency of } G \\ &= 0. \quad \square \end{aligned}$$

Thus, all projection maps in \mathcal{E}^n are symmetric idempotent matrices. So, if P_1 and P_2 are symmetric idempotent matrices, then they are both projection matrices onto linear subspaces. If $P_1P_2 = 0$, then the subspaces that P_1 and P_2 project onto are orthogonal. Now we see that the condition $P_1P_2 = 0$, which guarantees statistical independence of $y'P_1y$ and $y'P_2y$, for P_1, P_2 symmetric and idempotent matrices, makes sense. The reason is that we can write: $y'P_1y = (P_1y)'P_1y$ and $y'P_2y = (P_2y)'P_2y$, and P_1y and P_2y are those parts of the vector y that lie in the orthogonal subspaces $R(P_1)$ and $R(P_2)$. Because a multivariate normal density with covariance matrix σ^2I is spherically symmetric, these two pieces are statistically independent.

Suppose we define a linear subspace using the linear map or matrix X via $R(X) = \{v \in R^n : v = Xb, \text{ for some } b \in R^k\}$. What is the projection map onto $R(X)$? To answer this question, we need to define g -inverses, and in particular, the Moore–Penrose inverse.

A g -inverse of an $r \times s$ matrix H is any $s \times r$ matrix H^- such that

$$HH^-H = H.$$

Note that if the system of equations $Hx = b$ has a solution for given H and b , then $x = H^-b$ is a solution. This follows because if $Hx = b$ has a solution, then $b \in R(H)$, i.e., $b = Hw$ for some $w \in R^r$. In consequence, we obtain

$$\begin{aligned} Hx &= HH^-b = HH^-Hw, \\ &= Hw \\ &= b. \end{aligned}$$

For example, consider the normal equations for the least squares estimator $\hat{\beta}$: $X'X\hat{\beta} = X'y$. The solution is $\hat{\beta} = (X'X)^-X'y$. If $X'X$ is nonsingular, then $(X'X)^-$ is unique and equals $(X'X)^{-1}$.

If H is diagonal with less than full rank, i.e.,

$$H = \begin{bmatrix} h_1 & & & 0 \\ & \ddots & & \\ & & h_p & \\ 0 & & & 0 \end{bmatrix},$$

then any matrix of the form

$$\begin{bmatrix} h_1^{-1} & & 0 & H_2 \\ & \ddots & & \\ 0 & & h_p^{-1} & \\ H_3 & & & H_4 \end{bmatrix},$$

where H_2 , H_3 , and H_4 are arbitrary, is a g -inverse of H .

For a symmetric matrix A , we can find the totality of g -inverses of A by writing $A = B\Lambda B'$, where Λ is diagonal and B is orthogonal, and defining $A^- = B\Lambda^-B'$ for some g -inverse of Λ . All g -inverses of a diagonal matrix are of the form given above.

Note that $rk(H^-) \geq rk(H)$, where $rk(\cdot)$ denotes the rank of a matrix. This follows from the definition $HH^-H = H$. Also, there always exist full rank g -inverses. By placing additional conditions on the g -inverse, we can find g -inverses that have the same rank as the original matrix.

A g -inverse H^- is *reflexive* if it satisfies $H^-HH^- = H^-$.

Theorem 5: H^- is a reflexive g -inverse iff $rk(H^-) = rk(H)$.

Proof: See Rao and Mitra (1971) or Pringle and Rayner (1971). (The proof is easy, actually, at least in one direction.)

Definition: The Moore–Penrose inverse of a matrix, denoted H^+ , is a uniquely defined reflexive g -inverse that satisfies

$$(HH^+)' = HH^+ \text{ and } (H^+H)' = H^+H.$$

For example, the Moore–Penrose inverse of a non-zero scalar is its reciprocal. If the scalar is zero, the Moore–Penrose inverse is zero. Any number is a g -inverse of zero.

The Moore–Penrose inverse of a diagonal matrix $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p, 0, \dots, 0)$ is just $\Lambda^+ = \text{diag}(\lambda_1^{-1}, \dots, \lambda_p^{-1}, 0, \dots, 0)$. So, we can find the Moore–Penrose inverse of any matrix by diagonalization. (Use the singular value decomposition for non-square matrices.)

Theorem 6: The projection map onto $R(X)$ is $P_X = X(X'X)^-X'$ (for any choice of g -inverse of $X'X$).

Proof: We will show that $P_X y \in R(X)$ and $y - P_X y \perp R(X)$. Then, the projection theorem gives the result. Clearly, $P_X y \in R(X)$. To show $y - P_X y \perp R(X)$, write $y = y_1 + y_2$, where $y_1 \in R(X)$ and $y_2 \perp R(X)$. That is, $y = Xw + y_2$, for some $w \in R^k$. Consider any $b \in R(X)$. We can write $b = Xv$, for some $v \in R^k$, and we have

$$\begin{aligned}
b'(y - P_X y) &= v'X'(I - P_X)(Xw + y_2) \\
&= v'X'(I - P_X)Xw + v'X'(I - P_X)y_2 \\
&= v'[X'X - X'X(X'X)^-(X'X)]w + v'X'y_2 - v'X'X(X'X)^-X'y_2 \\
&= 0,
\end{aligned}$$

using the fact that $X'y_2 = 0$ because $y_2 \perp R(X)$. Thus, $y - P_X y \perp R(X)$. \square

So, if $y \in R^n$ and we want to project y onto the column space of X , i.e., we want to find the closest point in $R(X)$ to y , we have the answer: $X(X'X)^-X'y$.

The matrix $X(X'X)^-X'$ is the same no matter what g -inverse is used. This follows from the uniqueness of projections.

The final results for projection matrices onto $R(X)$ are the following:

Theorem 7: (a) $rk(P_X) = rk(X)$ and
(b) $rk(I - P_X) = n - rk(X)$, where X is an $n \times k$ matrix.

Proof: Since $P_X = X(X'X)^-X$ does not depend on the choice of g -inverse, we can use the Moore–Penrose inverse. Then, we have

$$\begin{aligned}
rk(P_X) &= \text{tr}(X(X'X)^+X') && \text{because } P_X \text{ is idempotent,} \\
&= \text{tr}(X'X(X'X)^+) && \text{by the properties of the trace,} \\
&= \text{tr}(B\Lambda B' B\Lambda^+ B') && \text{since } X'X = B\Lambda B', \\
&= \text{tr}(\Lambda\Lambda^+) \\
&= rk(\Lambda\Lambda^+) && \text{because } \Lambda\Lambda^+ \text{ is idempotent,} \\
&= rk(\Lambda) && \text{because } rk(\Lambda^+) \geq rk(\Lambda) \text{ and } \Lambda\Lambda^+\Lambda = \Lambda, \\
& && \text{i.e., } R(\Lambda^+) \supseteq R(\Lambda), \\
&= rk(X'X) && \text{because } X'X = B\Lambda B' \text{ and } B \text{ is full rank,} \\
&= rk(X) && \text{by known results.}
\end{aligned}$$

Also,

$$\begin{aligned}
rk(I - P_X) &= \text{tr}(I - P_X) && \text{because } I - P_X \text{ is idempotent,} \\
&= n - \text{tr}(P_X) \\
&= n - rk(X). && \square
\end{aligned}$$