

# LINEAR ALGEBRA

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## 0 Overview

## 1 the Normal equation

In this section, we'll refresh the reader on projections onto images of linear maps: The starting point of this construction is the following lemma:

**Lemma 1.1.** *Let  $W \subset V$  be a subspace of the inner product space  $V$ . Let  $v \in V$  and  $u \in W$ . Then the following are equivalent:*

1.  $(v - u) \perp W$
2.  $\operatorname{argmin}_{w \in W} \|v - w\| = u$

*Proof.* Let  $w \in W$ .

Assuming  $u \in W$  satisfies the first condition, we have  $v - u \perp u - w$  and by the Pythagorean theorem, we have:

$$\|v - w\|^2 = \|v - u\|^2 + \|u - w\|^2 \geq \|v - u\|^2$$

Proving the second condition.

Conversely, we assume  $u \in W$  satisfies the second condition and apply the following trick:

Consider the function:

$$\phi : \mathbb{R} \longrightarrow \mathbb{R} : t \mapsto \|v - u + tw\|^2$$

Since  $\|v - u\|^2$  is minimal,  $\phi$  has a minimum at  $t = 0$ . Moreover,  $\phi$  is differentiable so that  $\phi'(0) = 0$ . It's also easy to see that

$$\phi(t) = \|v - u\|^2 + 2 \cdot t \langle v - u, w \rangle + t^2 \|w\|^2$$

Hence  $0 = \phi'(0) = 2 \langle v - u, w \rangle$ , and  $v - u \perp w$  as required

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**Lemma 1.2.** *Let  $W \subset V$  be a subspace of a finite-dimensional inner product space. Then the map*

$$\pi : V \longrightarrow W : v \mapsto \operatorname{argmin}_{w \in W} \|v - w\|$$

*is well defined*

*Proof.* By the above lemma we need to show that for any  $v \in V$ , there exists a unique  $\pi(v) \in W$  such that  $v - \pi(v) \perp W$ . To this end, we look at the following map  $f \in W^*$

$$f : W \longrightarrow \mathbb{R} : w \mapsto \langle v, w \rangle$$

Since  $W^*$  is in turn an inner product space,  $f$  can be written in the form  $\langle \pi(v), - \rangle$  for some unique  $\pi(v) \in W$ . The result now follows X

The lemma above motivates the following definition:

**Definition 1.3.** Let  $W \subset V$  be a subspace of a finite dimensional inner product space. Then the unique map  $\pi : V \longrightarrow W$  defined by

$$\pi(v) \stackrel{\text{def}}{=} \operatorname{argmin}_{w \in W} \|v - w\|$$

*is the projection of  $V$  onto  $W$*

**Corollary 1.4.** *Let  $W = \operatorname{im}(f) \oplus \operatorname{im}(f)^\perp$  and  $\pi_{\operatorname{im}(f)} : W \longrightarrow \operatorname{im}(f)$  be the canonical projection. Then  $\pi_{\operatorname{im}(f)}$  coincides with the projection onto the subspace  $\operatorname{im}(f) \subset W$  in the sense of Definition 1.3*

*Proof.* This follows immediately from 1.1 X

Next, we consider a linear map  $f \in \operatorname{Hom}_{\mathbb{K}}(U, V)$  and let  $W$  be the subspace  $\operatorname{im}(f)$ . One can give a more explicit description of the projection  $\pi : V \longrightarrow W$ :

**Lemma 1.5.** *Let  $f \in \operatorname{Hom}(U, V)$  and  $v \in V$ . Then the following are equivalent:*

1.  $f(u)$  is the projection of  $v$  onto the subspace  $\operatorname{im}(f) \subset V$
2. The vector  $u \in U$  satisfies  $(f^* \circ f)(u) = f^*(v)$

*Proof.*  $f(u)$  is the projection of  $v$  onto  $\operatorname{im}(f)$  if and only if  $\langle v - f(u), f(u') \rangle = 0$  for any  $u' \in U$  by Lemma 1.1. Now,

$$\langle v - f(u), f(u') \rangle = \langle f^*(v) - f^*f(u), u' \rangle$$

This last expression is 0 if and only if  $f^*(v) - f^*f(u) = 0$  since the inner product is nondegenerate X

The above lemma justifies the following definition:

**Definition 1.6.** Let  $f \in \operatorname{Hom}(V, W)$  and  $w \in W$ .

We say that  $v \in V$  satisfies the normal equation if and only if

$$(f^* \circ f)(v) = f^*w$$

In this terminology, we can restate lemma 1.5 as follows:

**Lemma 1.7.** *Let  $f \in \operatorname{Hom}(V, W)$  and  $w \in W$ . Then the following are equivalent:*

1.  $w = \operatorname{argmin}_{u \in V} \|w - f(u)\|$
2.  $v$  is a solution to the normal equation  $(f^* \circ f)(v) = f^*w$

It is finding the solutions to this equation that we are interested in. It turns out that one can give an explicit description of them using the so-called *Moore-Penrose pseudo-inverse*. Since this construction seems to be a little less well covered in standard linear algebra literature, we'll discuss in detail below:

## 2 the (Moore-Penrose) Pseudo-inverse

In this section, we will let  $V, W$  be finite-dimensional vector spaces and  $f \in \text{Hom}_{\mathbb{R}}(V, W)$ .

It is well-known that  $f$  does not have an inverse in general. There is however a natural generalization of the notion of inverse which can be defined for *any* map: a *pseudo-inverse*. More precisely, if  $f$  either has a nonzero kernel or if the image of  $f$  is not the whole of  $W$ , then the inverse of  $f$  will not exist. One natural way to remediate this issue is to consider complements for both subspaces and write

$$V \stackrel{\text{def}}{=} \ker(f) \oplus U_V \text{ and } W \stackrel{\text{def}}{=} \text{im}(f) \oplus U_W$$

It's easy to see that restricting  $f$  to appropriate subspaces now does produce an invertible map as follows:

**Lemma 2.1.** *the map  $f : U_V \longrightarrow \text{im}(f)$  is an isomorphism.*

We'll denote the inverse of  $f$  on  $U_V$  by  $f^\sharp : \text{im}(f) \longrightarrow U_V$ . A pseudo-inverse is now the natural lift of  $f^\sharp$  to the whole of  $W$ :

**Lemma 2.2.** *There exists a unique map  $f^\sharp : W \longrightarrow U_V$  making the following diagram commute:*

$$\begin{array}{ccc} W & & \\ \pi_{\text{im}(f)} \downarrow & \searrow f^\sharp & \\ \text{im}(f) & \xrightarrow{f^\sharp} & U_V \end{array}$$

*Proof.* The commutativity of the diagram means that for  $u \in U_V$ , we have

$$f^\sharp(w) \stackrel{\text{def}}{=} u \iff f^\sharp(\pi_{\text{im}(f)}(w)) = u \iff \pi_{\text{im}(f)}(w) = f(u)$$

Where the second equivalence follows from the fact that  $f^\sharp$  is the inver of  $f$  on  $U_V$ .

The claim will thus follow if we show that the above assignment is indeed a well-defined linear map. To this end assume that  $u, u' \in U_V$  satisfy  $f(u') = \pi_{\text{im}(f)}(w) = f(u)$ .

Then  $u - u' \in \ker(f)$ , hence  $u - u' \in \ker(f) \cap U_V$  in particular. Now since  $\ker(f) \oplus U_V = V$ , we have  $u - u' = 0$ , so that  $u = u'$ , showing the well-definedness.

We leave the linearity to the reader. X

It will be helpful to note that the map  $f^\sharp \in \text{Hom}(W, V)$  can also be characterized by  $\text{im}(f^\sharp) \subset U_V$  and  $f \circ f^\sharp = \pi_{\text{im}(f)}$ .

To give the map  $f^\sharp$  a name, we first let  $\Lambda(f)$  denote the set

$$\Lambda(f) \stackrel{\text{def}}{=} \{(U_V, U_W) \mid \ker(f) \oplus U_V = V \text{ and } \text{im}(f) \oplus U_W = W\}$$

and conclude from Lemma 2.2 that there is a assignment:

$$\Phi : \Lambda(f) \longrightarrow \text{Hom}_{\mathbb{R}}(W, V) : (U_V, U_W) \mapsto f^\sharp$$

where  $f^\sharp \in \text{Hom}_{\mathbb{R}}(W, V)$  is the unique map satisfying

$$f \circ f^\sharp = \pi_{\text{im}(f)} \text{ and } \text{im}(f^\sharp) \subset U_V$$

Let's denote the image of  $\Phi$  by  $\Pi(f)$ . Summarizing the discussion, we make the following:

**Definition 2.3.** Let  $(U_V, U_W) \in \Lambda(f)$ . Then the pseudo-inverse of  $(U_V, U_W, f)$  is the map  $\Phi(f)$ .

We say that  $g \in \text{Hom}_{\mathbb{R}}(W, V)$  is a pseudo-inverse to  $f$  if  $g \in \Pi(f)$

We can give a slightly different description of pseudo-inverses by describing them on the 2 components in the decomposition  $\text{im}(f) \oplus U_W = W$ :

**Lemma 2.4.** *Let  $(U_V, U_W)$  in  $\Lambda(f)$ . Then the following are equivalent:*

1.  $f^\sharp$  is the pseudo-inverse to  $(U_V, U_W, f)$
2.  $f^\sharp|_{\text{im}(f)}$  is the inverse to  $f : U_V \longrightarrow \text{im}(f)$  and  $f^\sharp|_{U_W} = 0$

*Proof.* Since the pseudo-inverse to  $(U_V, U_W, f)$  is unique, it suffices to show that the pseudo-inverse indeed satisfies the conditions of (2). The fact that  $f^\sharp|_{\text{im}(f)}$  is the inverse of  $f|_{U_V}$  follows from

$$(f \circ f^\sharp)|_{\text{im}(f)} = (\pi_{\text{im}(f)})|_{\text{im}(f)} = \text{Id}|_{\text{im}(f)}$$

Moreover, if  $w \in U_W$ , then  $\pi_{\text{im}(f)}(w) = 0$  since  $\text{im}(f) \oplus U_W$ . Hence  $f^\sharp(w) = f^\sharp(\pi_{\text{im}(f)}(w)) = 0$  by Lemma 2.2 X

Our next order of business is to give an explicit description of the set  $\Pi(f)$  of pseudo-inverses to  $f$ . We begin by showing that we can describe the complements  $U_V$  and  $U_W$  solely by using the maps  $f$  and  $f^\sharp$ :

**Lemma 2.5.** *Let  $f^\sharp$  be the pseudo-inverse to  $(U_V, U_W, f)$ . Then  $U_V = \text{im}(f^\sharp)$  and  $U_W = \ker(f^\sharp)$*

*Proof.* We have  $\text{im}(f^\sharp) \subset U_V$  by Definition 2.3. Moreover,  $f^\sharp$  is a composition of surjections and hence itself surjective, proving the first claim.

To prove the second claim, note that the second condition of Lemma 2.4 immediately implies that  $U_W \subset \ker(f^\sharp)$ . We can also show the other inclusion by assuming that  $w \in W$  satisfies  $f^\sharp(w) = 0$ , in which case  $\pi_{\text{im}(f)}(w) = f(f^\sharp(w)) = f(0) = 0$ , implying that  $w$  lies in the component  $U_W$  of the decomposition  $\text{im}(f) \oplus U_W = W$  as required X

Taking the above lemma one step further allows us to describe the set  $\Pi(f)$  of pseudo-inverses as promised:

**Lemma 2.6.** *Let  $f \in \text{Hom}(V, W)$ . Then the following are equivalent:*

1.  $g \in \Pi(f)$
2.  $(f \circ g)|_{\text{im}(f)} = \text{Id}$  and  $(g \circ f)|_{\text{im}(g)} = \text{Id}$

*Proof.* Let  $g$  be a pseudo-inverse to  $f$  and define  $U_V \stackrel{\text{def}}{=} \text{im}(g)$  and  $U_W \stackrel{\text{def}}{=} \ker(f)$ . Then Lemma 2.5 shows that  $g$  is in fact the pseudo-inverse to the triple  $(U_V, U_W, f)$ . Now, since  $g|_{\text{im}(f)}$  is the inverse to  $f|_{U_V}$  by Lemma 2.4, we have  $(f \circ g)|_{\text{im}(f)} = \text{Id}$  and  $(g \circ f)|_{\text{im}(g)} = (g \circ f)|_{U_V} = \text{Id}$ .

Conversely, assume that  $g$  satisfies the conditions in (2).

We begin by showing that  $(\text{im}(g), \ker(g)) \in \Lambda(f)$ . Let's show that  $\text{im}(f) \oplus \ker(g) = W$  by way of example. Indeed, first note that  $\text{im}(f) \cap \ker(g) = 0$ , as any  $w$  in this intersection must satisfy  $w = (f \circ g)(w) = f(0) = 0$ . Moreover, if we write  $w = (w - f(g(w))) + f(g(w))$ , we see that trivially  $f(g(w)) \in \text{im}(f)$  and

$$g(w - f(g(w))) = g(w) - (g(f(g(w))) = g(w) - g(w) = 0$$

so that  $(w - f(g(w))) \in \ker(g)$ . This indeed shows that  $\text{im}(f) \oplus \ker(g) = W$ . The proof of  $\text{im}(g) \oplus \ker(f) = V$  is completely analogous, allowing us to conclude that  $(\text{im}(g), \ker(g)) \in \Lambda(f)$ .

It now remains to show that  $g$  is indeed a pseudo-inverse to the triple  $(\text{im}(g), \ker(f), f)$ . By Lemma 2.4, it suffices to show that  $g|_{\text{im}(f)}$  is the inverse to  $f|_{\text{im}(g)}$  and that  $g|_{\ker(f)} = 0$ . The first claim follows immediately from the fact that  $g$  is a left inverse to  $f : \text{im}(g) \longrightarrow W$  and the second claim is trivial. X

In order to summarize the previous 2 lemmas, we introduce the following assignment, which is well-defined by Lemma 2.5

$$\Psi : \Pi(f) \longrightarrow \Lambda(f) : g \mapsto (\text{im}(g), \ker(g))$$

We now have:

**Lemma 2.7.** *Let  $f \in \text{Hom}(V, W)$ . Then:*

- $\Pi(f) = \{g \in \text{Hom}(W, V) \mid (f \circ g)|_{\text{im}(f)} = \text{Id} \text{ and } (g \circ f)|_{\text{im}(g)} = \text{Id}\}$
- *The assignments  $\Phi$  and  $\Psi$  define 1:1 correspondences between  $\Lambda(f)$  and  $\Pi(f)$*

*Proof.* The first claim simply restates Lemma 2.6. To prove the second, we note that  $\Psi \circ \Phi = \text{Id}$  by Lemma 2.5. Moreover,  $\Phi$  is surjective by definition, implying that  $\Phi \circ \Psi = \text{Id}$  as well X

We finish our discussion of pseudo-inverses by discussing a special choice of pseudo-inverse in  $\Pi(f)$  that one can make if the vector spaces  $V$  and  $W$  are equipped with inner products. Indeed, recall the following standard result:

**Lemma 2.8.** *Let  $U \subset V$  be a subspace of a finite dimensional inner product space. Then  $U \oplus U^\perp = V$*

This leads us to the following Definition:

**Definition 2.9.** Let  $V, W$  be finite-dimensional inner product spaces and let  $f \in \text{Hom}_{\mathbb{R}}(V, W)$ . Then the *Moore-Penrose pseudo-inverse* is the pseudo-inverse to the triple  $(\ker(f)^\perp, \text{im}(f)^\perp, f)$ .

We will denote it by  $f^+$

It turns out that we can give a very satisfying description of Moore-Penrose pseudo-inverses:

**Lemma 2.10.** *Let  $V, W$  be finite-dimensional inner product spaces and  $f \in \text{Hom}(V, W)$ . Then the following are equivalent:*

1.  *$g$  is the Moore-Penrose pseudo-inverse  $f^+$  to  $f$*
2.  *$g$  is a pseudo-inverse to  $f$  and  $g \circ f$  and  $f \circ g$  are self-adjoint linear maps*
3.  *$f$  and  $g$  satisfy  $f \circ g \circ f = f$ ,  $g \circ f \circ g = g$ ,  $(g \circ f)^* = g \circ f$  and  $(f \circ g)^* = f \circ g$*

*Proof.* The equivalence (2)  $\iff$  (3) is simply a restatement of Lemma 2.7.

We now prove (2)  $\implies$  (1):

Assume that  $g$  is a pseudo-inverse to  $f$  and that  $g \circ f$  and  $f \circ g$  are both self-adjoint. then Lemma 2.5 implies that  $g$  is the pseudo-inverse to the triple  $(\text{im}(g), \ker(f), f)$ . The claim will thus follow if we show that  $\text{im}(g) = \ker(f)^\perp$  and  $\ker(g) = \text{im}(f)^\perp$ . By way of example, we will prove the former equality: First note that since  $\text{im}(g) \oplus \ker(f) = V$ , it suffices to show that  $\text{im}(g) \perp \ker(f)$ . Indeed, for  $w \in W$  and  $v \in \ker(f)$ , we have:

$$\langle v, g(w) \rangle = \langle v, (g \circ f)(g(w)) \rangle = \langle (g \circ f)^*(v), g(w) \rangle = \langle (g \circ f)(v), g(w) \rangle = \langle g(0), g(w) \rangle = 0$$

The proof of  $\ker(g) = \text{im}(f)^\perp$  is analogous.

Finally, we show (1)  $\implies$  (2):

Assume that  $g$  is the Moore Penrose pseudo-inverse to  $f$ . Ie  $g$  is the pseudo-inverse to the triple  $(\ker(f)^\perp, \text{im}(f)^\perp, f)$ .

We will show that  $(f \circ g)$  is self-adjoint and leave the other claim to the reader. To this end, let  $v, v' \in V$ .

Then

$$\begin{aligned} \langle v, g(f(v')) \rangle &= \left\langle v - g(f(v)) + g(f(v)), g(f(v')) - v' + v' \right\rangle \\ &= \left\langle v - g(f(v)), g(f(v')) \right\rangle + \left\langle g(f(v)), g(f(v')) - v' \right\rangle + \left\langle g(f(v)), v' \right\rangle \end{aligned}$$

Now, since  $f \circ g \circ f = f$ , we conclude that  $v - g(f(v))$  and  $g(f(v')) - v'$  lie in  $\ker(f)$ . Moreover, since  $\ker(f) = \text{im}(g)^\perp$ , we conclude that

$$\langle v - g(f(v)), g(f(v')) \rangle = \langle g(f(v)), g(f(v')) - v' \rangle = 0$$

So that

$$\langle v, g(f(v')) \rangle = \langle g(f(v)), v' \rangle$$

implying that  $f \circ g = (f \circ g)^*$ . The equality  $g \circ f = (g \circ f)^*$  is completely analogous. X

As mentioned in the introduction of this section, our main motivation for studying the Moore-Penrose pseudo-inverse, is to provide a description of the projection of a vector onto the image of a linear map. We begin with the following preparatory lemma:

**Lemma 2.11.** *Let  $V, W$  be finite-dimensional inner product spaces and  $f \in \text{Hom}(V, W)$ . Let  $v \in V$  and  $w \in W$ . Finally denote the Moore-Penrose inverse of  $f$  by  $f^+$ . Then the following are equivalent:*

1.  $f(v)$  is the projection of  $w$  onto the subspace  $\text{im}(f)$
2.  $v$  satisfies the normal equation  $(f^* \circ f)(v) = f^*(w)$
3.  $v$  lies in the affine subspace  $f^+(w) + \ker(f)$

*Proof.* The equivalence of (1)  $\iff$  (2) is simply a restatement of Lemma 1.5.

To show the equivalence of (1)  $\iff$  (3), we first note that  $f(f^+w) = \pi_{\text{im}(f)}(w)$ , where  $\pi_{\text{im}(f)}$  is the projection onto the subspace  $\text{im}(f) \subset W$  by Lemma 1.4. This shows that the vector  $f^+(w) \in V$  indeed satisfies the condition (1). Next, assume (1), so that  $v \in V$  satisfies  $f(v) = \pi_{\text{im}(f)}(w)$  and write  $v = f^+(w) + v'$ . Then

$$f(v) = \pi_{\text{im}(f)}(w) \iff f(f^+(w) + v') = \pi_{\text{im}(f)}(w) \iff \pi_{\text{im}(f)}(w) + f(v') = \pi_{\text{im}(f)}(w) \iff v' \in \ker(f)$$

This proves the claim X

This lemma has an interesting corollary which allows us to write the Moore-Penrose even more explicitly which will play an important role later on:

**Corollary 2.12.** *Let  $V$  be a finite dimensional vector space and  $W$  a finite dimensional inner product space. Let  $f \in \text{Hom}(V, W)$  be injective and choose any inner product on  $V$ . Then*

$$f^+ = (f^* \circ f)^{-1} \circ f^*$$

*Proof.* Since  $f$  is injective (so that  $\ker(f) = 0$ ),  $f^+$  is the pseudo-inverse to the triple  $(V, \text{im}(f)^\perp, f)$  by Definition 2.9. It follows immediately that this condition is independent of the inner product on  $V$ . To prove the formula, simply note that  $f^* \circ f$  is invertible if  $f$  is injective and apply the second criterium of Lemma 2.11 X

## 3 Principal Component Analysis

**3.1. the Principal component basis** Throughout this section  $V$  will denote a fd. Euclidean space with inner product  $\langle -, - \rangle$ . We will also consider a finite subset  $\Delta \subset V$  of *data*. The goal of this section is to exhibit an orthonormal basis for  $V$  which fits the data *suitably*. We begin by defining the principal components of  $\Delta$ , a specific choice of lines which span an orthonormal basis particularly compatible with  $\Delta$ .

To make our exposition clearer, we introduce the notation  $\langle \Delta, u \rangle \stackrel{\text{def}}{=} \{\langle x, u \rangle\}_{x \in \Delta} \in \mathbb{R}^\Delta$ . Recall from Probability (TODO) that  $\Delta$  defines the random variable  $1_\Delta : V \rightarrow \mathbb{R}$  whose pushforward probability is the sample probability on  $\mathbb{R}$ . Moreover, we can also consider the following random variable

$$X_u \stackrel{\text{def}}{=} V \rightarrow \mathbb{R} : x \mapsto \langle x, u \rangle \cdot 1_\Delta$$

Whose pushforward probability is the explained probability. More generally, we will prefix the different probabilistic concepts pertaining to this RV with the word *explained*.

We begin by constructing the first principal component, whose existence is guaranteed by the following theorem:

**Theorem 3.1.** *Let  $\bar{\Delta} = \frac{1}{|\Delta|} \sum_{x \in \Delta} x$  and let  $L$  be the set of lines through  $\bar{\Delta}$  in  $V$ . Then there is a unique line  $\ell \in L$  minimizing*

$$\sum_{x \in \Delta} \|x - \pi_{\ell}(x)\|^2$$

*Moreover, if we write  $\ell = \bar{\Delta} + \mathbb{R}u$  with  $\|u\| = 1$ , then the above three quantities coincide:*

- $\sum_{x \in \Delta} \|x - \pi_{\ell}(x)\|^2$
- the explained variance of  $X_u$
- The largest eigenvalue of  $M^t \cdot M$  where  $\phi : V \rightarrow \mathbb{R}^{\Delta}$  is given by  $\phi(u) = \langle \Delta, u \rangle$

**Definition 3.2.** The principal component of  $\Delta$  is the line  $\ell \in L$  defined in the above theorem

**Lemma 3.3.** *Let  $\ell = \mathbb{R}u$  where  $\|u\| = 1$ . Then the following are equivalent:*

- The mean square error  $\sum_{x \in \Delta} \|x - \pi_{\ell}(x)\|^2$  is minimal
- $\sum_{x \in \Delta} \langle x, u \rangle^2$  is minimal

## 3.2. Application: Dimension Reduction

*Proof.* This is an easy exercise in bilinear forms

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**Remark 3.4.** *Note that if  $\bar{\Delta} = 0$  (an assumption commonly made in ML), then the latter quantity is the explained variance of  $\Delta$  in our terminology.*

For the next lemma we recall that the spectral theorem tells us that a symmetric endomorphism always has basis of eigenvectors which can be chosen to be orthonormal.

**Lemma 3.5.** *Assume  $\bar{\Delta} = 0$ . Consider the linear map*

$$\phi : V \rightarrow \mathbb{R}^{\Delta} : u \mapsto \langle \Delta, u \rangle$$

*Let  $u_1, \dots, u_n$  be an orthormal basis of eigenvectors for  $\phi^t \circ \phi \in \text{End}_{\mathbb{R}}(V)$ . Then*

- The eigenvalue for  $u_i$  is  $\lambda_i \stackrel{\text{def}}{=} \sum_{x \in \Delta} \langle x, u_i \rangle^2$
- $\sup_{u \in B(0,1)} \sum_{x \in \Delta} \langle x, u \rangle^2 = \max_i \{\lambda_i\}$

*Proof.* Let  $u \in V$ . Then the explained variance of  $\Delta$  with respect to  $u$  is

$$\sum_{x \in \Delta} \langle x, u \rangle^2 = \|\phi(u)\|_{\mathbb{R}^{\Delta}}^2 = \langle \phi(u), \phi(u) \rangle = \langle u, (\phi^t \circ \phi)(u) \rangle$$

Writing  $u \stackrel{\text{def}}{=} \sum \alpha_i u_i$  wrt the orthonormal basis of eigenvectors then yields

$$\sum_{x \in \Delta} \langle x, u \rangle^2 = \langle u, (\phi^t \circ \phi)(u) \rangle = \left\langle \sum \alpha_i u_i, (\phi^t \circ \phi) \left( \sum \alpha_i u_i \right) \right\rangle = \left\langle \sum \alpha_i u_i, \left( \sum \lambda_i \alpha_i u_i \right) \right\rangle = \sum_i \lambda_i \alpha_i^2$$

In particular if  $u = u_i$ , we obtain the first claim. To prove the second, we assume additionally that  $u \in B(0,1)$  and let  $\lambda_n$  be the largest eigenvalue. Then

$$\sum_{x \in \Delta} \langle x, u \rangle^2 = \sum_i \lambda_i \alpha_i^2 \leq \lambda_n \sum_i \alpha_i^2 = \lambda_n$$

And this value indeed gets reached by  $u_n$

X

*proof of Theorem 3.1.* First we claim that wlog we can assume that  $\bar{\Delta} = 0$ . Indeed

Next, by Lemma 3.3, we need to maximize the explained variance  $\sum_{x \in \Delta} \langle x, u \rangle^2$  which by lemma 3.5 coincides with the largest eigenvalue. The line  $\ell$  is now spanned by any corresponding eigenvector. X

Since the endomorphism  $\mathcal{L} \stackrel{\text{def}}{=} \phi^t \circ \phi$  plays a crucial role in our discussion, we give a more explicit description:

**Lemma 3.6.** *The map  $\mathcal{L}^t : \mathbb{R}^n \longrightarrow \mathbb{R}^n$  is given by the matrix whose  $(i, j)$ -component is  $\langle x_i, u_j \rangle$ .*

*Proof.* Let  $M$  be said matrix. Then the  $j$ -th column is given by  $M \cdot e_j$  (where  $e_j$  is of course the  $j^{\text{th}}$  standard basisvector for  $\mathbb{R}^n$ ). X

**Definition 3.7.** the principal component basis of  $\Delta$  is the orthonormal basis of eigenvectors for the map  $\mathcal{L}$ .

**3.3. Application: Dimension Reduction** One can use PCA to find a way to reduce the dimension of the dataspace:

**Definition 3.8.** The reduction of order  $n$  of the dataset  $\Delta \subset V$  is the image of the map

**Definition 3.9.** The pc reconstruction of order  $n$  of the dataset  $\Delta$  is