

# COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2024.

Lecture 14

- Midterms and Problem Set 2 are being graded now.
- Problem Set 3 will be released shortly, likely due 11/8.
- Quiz due monday.

# Summary

## Last Few Classes: The Johnson-Lindenstrauss Lemma

- Reduce  $n$  data points in **any dimension  $d$**  to  $O\left(\frac{\log n}{\epsilon^2}\right)$  dimensions and preserve **all pairwise distances** up to  $1 \pm \epsilon$ .
- **Compression is linear** via multiplication with a random, **data oblivious**, matrix (linear compression)  $[ \pi ] [x] \rightarrow [x]$
- Proved via the distributional JL-Lemma which shows that if  $\Pi \in \mathbb{R}^{m \times d}$  is a random matrix,  $\|\Pi \vec{y}\|_2 \approx \|\vec{y}\|$  for any  $y$  with high probability.  $y = x_i - x_j$
- Proof of distributional JL via linearity of expectation, linearity of variance, stability of the Gaussian distribution, and an exponential concentration bound for Chi-Squared random variables.

# Summary

Next Few Classes: Low-rank approximation, the SVD, and principal component analysis (PCA).

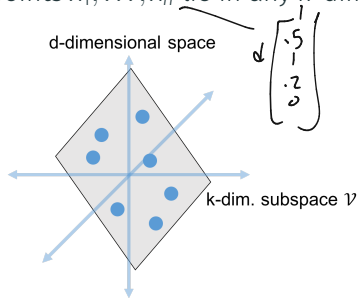
$$\begin{bmatrix} \uparrow \\ \uparrow \\ \uparrow \end{bmatrix} \rightarrow_m \begin{bmatrix} \uparrow \\ \uparrow \end{bmatrix}$$

- Reduce  $d$ -dimensional data points to a smaller dimension  $m$ .
- Like JL, **compression is linear** – by applying a matrix.
- Chose this matrix carefully, taking into account **structure of the dataset**.
- Can give better compression than random projection (although not directly comparable).

Will be using a fair amount of linear algebra: orthogonal basis, column/row span, eigenvectors, etc.

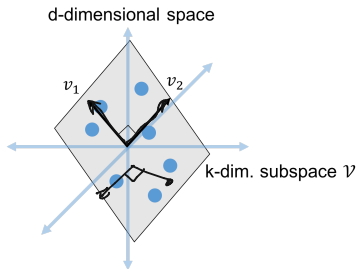
# Embedding with Assumptions

Assume that data points  $\vec{x}_1, \dots, \vec{x}_n$  lie in any  $k$ -dimensional subspace  $\mathcal{V}$  of  $\mathbb{R}^d$ .



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Claim: Let  $\vec{v}_1, \dots, \vec{v}_k$  be an orthonormal basis for  $\mathcal{V}$  and  $\mathbf{V} \in \mathbb{R}^{d \times k}$  be the matrix with these vectors as its columns. For all  $\vec{x}_i, \vec{x}_j$ :

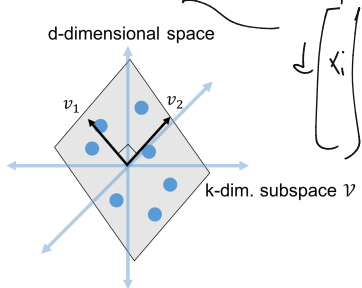
$$\mathbf{V} = \begin{matrix} & \begin{matrix} \downarrow & \downarrow & \downarrow & \dots \end{matrix} \\ \begin{matrix} \downarrow \\ \downarrow \\ \downarrow \\ \dots \end{matrix} & \begin{bmatrix} | & | & | & \dots \\ v_1 & v_2 & v_3 & \dots \\ | & | & | & \dots \\ | & | & | & \dots \\ | & | & | & \dots \end{bmatrix} \end{matrix}$$

$$\underbrace{\|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2}_{\mathbb{R}^k} = \|\vec{x}_i - \vec{x}_j\|_2$$

$\mathbb{R}^d$

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$$\|\Pi \vec{x}_i - \Pi \vec{x}_j\|$$

$$\|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2 = \|\vec{x}_i - \vec{x}_j\|_2.$$

- $\mathbf{V}^T \in \mathbb{R}^{k \times d}$  is a linear embedding of  $\vec{x}_1, \dots, \vec{x}_n$  into  $k$  dimensions with no distortion.

# Dot Product Transformation

**Claim:** Let  $\vec{v}_1, \dots, \vec{v}_k$  be an orthonormal basis for  $\mathcal{V}$  and  $V \in \mathbb{R}^{d \times k}$  be the matrix with these vectors as its columns. For all  $\vec{x}_i, \vec{x}_j \in \mathcal{V}$ :

$$\|V^T \vec{x}_i - V^T \vec{x}_j\|_2 = \|\vec{x}_i - \vec{x}_j\|_2.$$

for all  $i, j$   $\exists c_i \in \mathbb{R}^k$

$$\begin{bmatrix} \vec{x}_i \\ \vdots \\ \vec{x}_j \end{bmatrix} = \begin{bmatrix} V \\ \vdots \\ V \end{bmatrix} \begin{bmatrix} c_i \\ \vdots \\ c_j \end{bmatrix}$$

$$x_i = V c_i$$

$$x_i = \vec{v}_1 \cdot c_i(1) + \vec{v}_2 \cdot c_i(2) \dots + \vec{v}_k \cdot c_i(k)$$

$$\|V^T x_i - V^T x_j\|_2^2$$

$$= \| \underbrace{V^T V}_{I} c_i - V^T V c_j \|_2^2 = \| c_i - c_j \|_2^2$$

$$(V^T V)_{ij} = \langle v_i, v_j \rangle = v_i^T v_j$$

$$= \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i \neq j \end{cases}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ \vdots & \vdots \end{bmatrix}$$

$$\|V c_i - V c_j\|_2^2$$

$$= \langle V(c_i - c_j), V(c_i - c_j) \rangle$$

$$= (c_i - c_j)^T \underbrace{V^T V}_{I} (c_i - c_j)$$

$$(c_i - c_j)^T (c_i - c_j)$$

$$\|c_i - c_j\|_2^2$$

$$\|y\|_2 = \sqrt{\sum y_i^2}$$

$$\|y\|_2^2 = \sum y_i^2$$

$$= \langle y, y \rangle$$

$$= y^T y$$



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$$\|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2 = \|\vec{x}_i - \vec{x}_j\|_2.$$

$$\|y\|_2 = \sqrt{\sum_{i=1}^d y(i)^2}$$

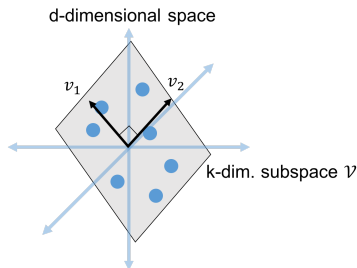
$$\|y\|_2^2 = \sum_{i=1}^d y(i)^2 = \langle y, y \rangle$$

$$\left( \sum_{i=1}^d y(i) \cdot y(i) \right) = \sum_{i=1}^d y(i)^2$$

$$1 \cdot \begin{pmatrix} y \\ \vdots \\ y \end{pmatrix}^T \begin{pmatrix} y \\ \vdots \\ y \end{pmatrix} = \sum_{i=1}^d y(i)^2$$

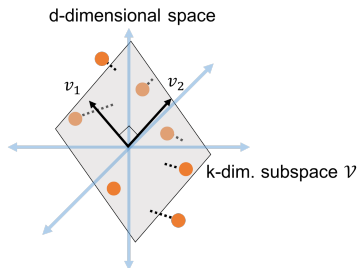
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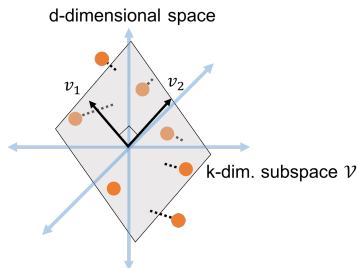
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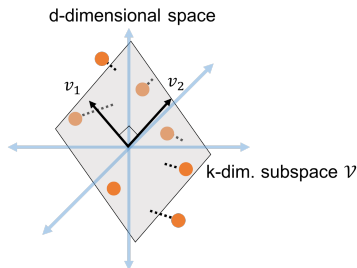
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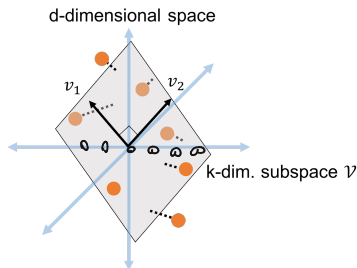
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- How do we find  $\mathcal{V}$  and  $\mathbf{V}$ ?
- How good is the embedding?

# Low-Rank Factorization

**Claim:**  $\vec{x}_1, \dots, \vec{x}_n$  lie in a  $k$ -dimensional subspace  $\mathcal{V} \Leftrightarrow$  the data matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  has  $\text{rank} \leq k$ .

$$\mathbf{X} = \begin{bmatrix} \text{---} & \overset{d}{x_1^T} & \text{---} \\ & x_2^T & \\ & \vdots & \\ & \vdots & \\ \text{---} & x_n^T & \text{---} \end{bmatrix} \quad \text{rank}(\mathbf{X}) \leq k$$

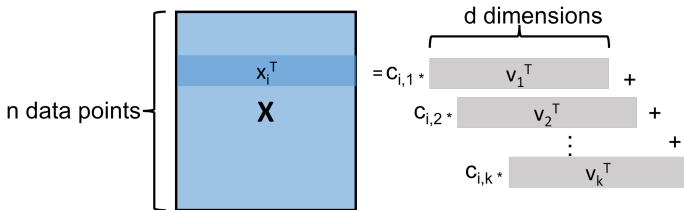
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- Letting  $\vec{v}_1, \dots, \vec{v}_k$  be an orthonormal basis for  $\mathcal{V}$ , can write  $\vec{x}_i$  as:

$$\vec{x}_i = \mathbf{V}\vec{c}_i = c_{i,1} \cdot \vec{v}_1 + c_{i,2} \cdot \vec{v}_2 + \dots + c_{i,k} \cdot \vec{v}_k.$$



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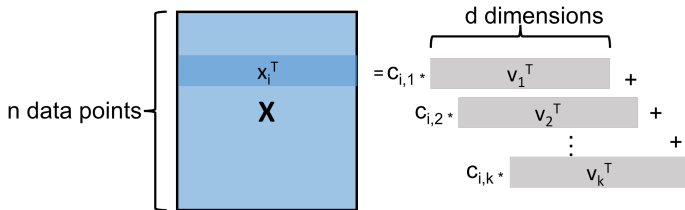
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- So  $\vec{v}_1, \dots, \vec{v}_k$  span the rows of  $\mathbf{X}$  and thus  $\text{rank}(\mathbf{X}) \leq k$ .



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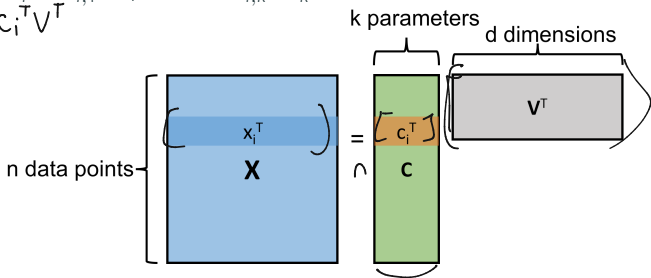
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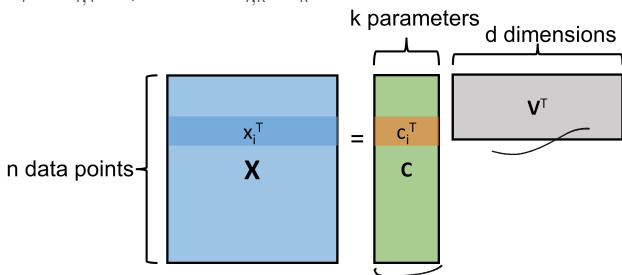
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*rank(X) = 2*

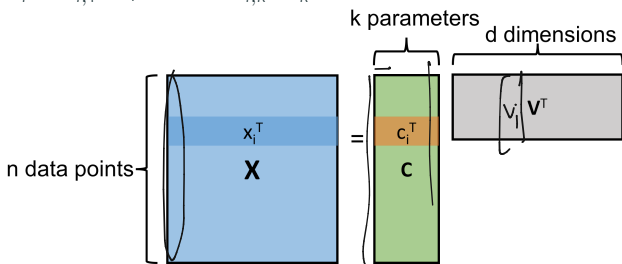


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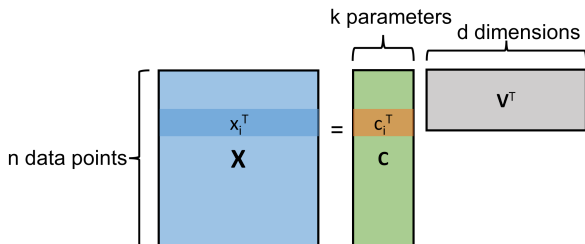


- $\mathbf{X}$  can be represented by  $(n + d) \cdot k$  parameters vs.  $n \cdot d$ .
- The rows of  $\mathbf{X}$  are spanned by  $k$  vectors: the columns of  $\mathbf{V} \implies$  the columns of  $\mathbf{X}$  are spanned by  $k$  vectors: the columns of  $\mathbf{C}$ .

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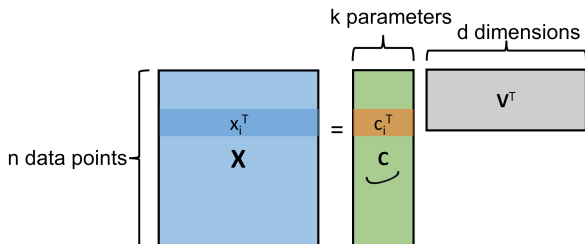
**Claim:** If  $\vec{x}_1, \dots, \vec{x}_n$  lie in a  $k$ -dimensional subspace with orthonormal basis  $\mathbf{V} \in \mathbb{R}^{d \times k}$ , the data matrix can be written as  $\mathbf{X} = \mathbf{C}\mathbf{V}^T$ .



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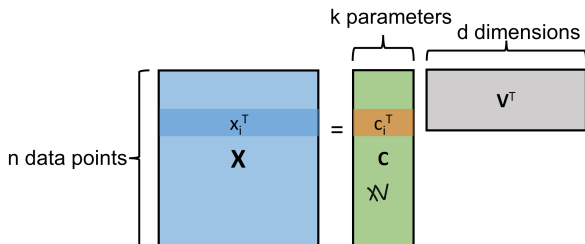
**Exercise:** What is this coefficient matrix  $\mathbf{C}$ ? **Hint:** Use that  $\mathbf{V}^T\mathbf{V} = \mathbf{I}$ .

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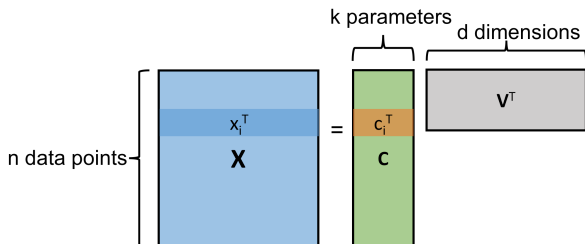
$$\mathbf{X}\mathbf{V} = \mathbf{C}\mathbf{V}^T\mathbf{V} \implies \mathbf{X}\mathbf{V} = \mathbf{C}\overset{\mathbf{I}}{\mathbf{V}^T\mathbf{V}} = \mathbf{C}$$

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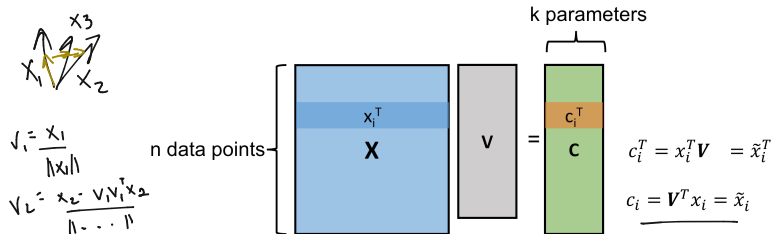
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$$\cdot \mathbf{X} = \mathbf{C}\mathbf{V}^T \implies \mathbf{X}\mathbf{V} = \mathbf{C}\mathbf{V}^T\mathbf{V} \implies \mathbf{X}\mathbf{V} = \mathbf{C}$$

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**Claim:** If  $\vec{x}_1, \dots, \vec{x}_n$  lie in a  $k$ -dimensional subspace  $\mathcal{V}$  with orthonormal basis  $\mathbf{V} \in \mathbb{R}^{d \times k}$ , the data matrix can be written as

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└ X V

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$$\begin{bmatrix} \mathbf{V} \end{bmatrix} \begin{bmatrix} \mathbf{V}^T \end{bmatrix} = \begin{bmatrix} \mathbf{W}^T \end{bmatrix}$$

$$\mathbf{X} = \mathbf{X} \mathbf{V} \mathbf{V}^T$$

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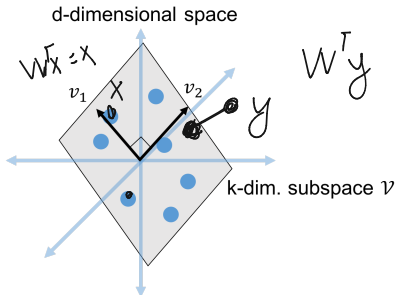
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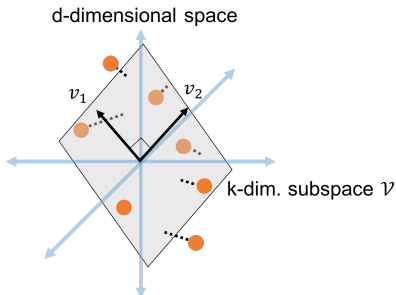
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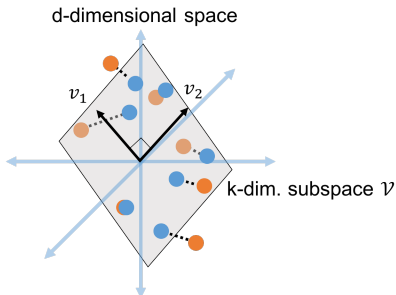
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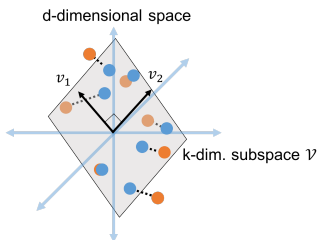
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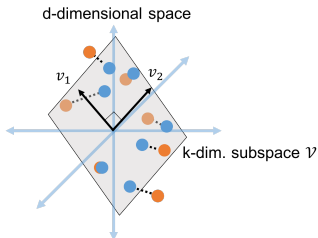


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$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$



$$n \begin{bmatrix} k & k \times d \\ \mathbf{V} & \mathbf{V}^T \end{bmatrix}$$

**Note:**  $\mathbf{X}\mathbf{V}\mathbf{V}^T$  has rank  $k$ . It is a **low-rank approximation** of  $\mathbf{X}$ .

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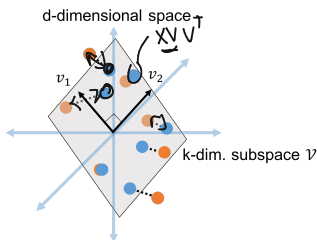
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$$\begin{bmatrix} x_{i1} & \dots & x_{id} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{nd} \end{bmatrix} \begin{bmatrix} v_1 & \dots & v_k \\ \vdots & & \vdots \\ v_1 & \dots & v_k \end{bmatrix}$$

$x_i^T \mathbf{V} \mathbf{V}^T$



$$\begin{aligned} \|\mathbf{X} - \mathbf{B}\|_F^2 &= \sum_{i,j} (x_{i,j} - b_{i,j})^2 \\ &= \sum_{i=1}^n \|x_i - b_i\|_2^2 \end{aligned}$$

*definition*

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$$\mathbf{XV}\mathbf{V}^T = \arg \min_{\mathbf{B} \text{ with rows in } \mathcal{V}} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (x_{i,j} - b_{i,j})^2 = \sum_i \|x_i - b_i\|_2^2$$

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$c_i \quad c_j \quad \|c_i - c_j\|_2$

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Key question is how to find the subspace  $\mathcal{V}$  and correspondingly  $\mathbf{V}$ .

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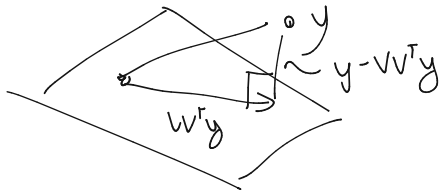
# Properties of Projection Matrices

**Quick Exercise:** Show that  $\mathbf{V}\mathbf{V}^T$  is **idempotent**. I.e.,  $(\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T)\vec{y} = (\mathbf{V}\mathbf{V}^T)\vec{y}$  for any  $\vec{y} \in \mathbb{R}^d$ .

Why does this make sense intuitively?

**Less Quick Exercise: (Pythagorean Theorem)** Show that:

$$\|\vec{y}\|_2^2 = \|(\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2 + \|\vec{y} - (\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2.$$



$$\mathbf{V}^T \mathbf{V} = \mathbf{I}$$



## A Step Back: Why Low-Rank Approximation?

**Question:** Why might we expect  $\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$  to lie close to a  $k$ -dimensional subspace?

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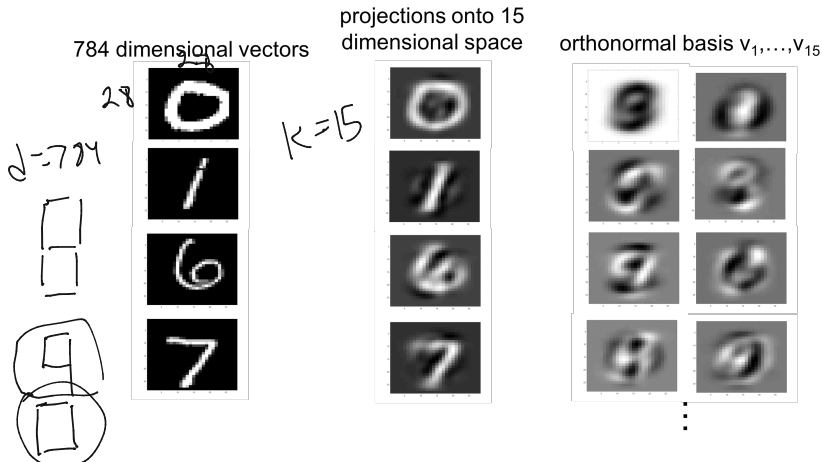
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home 2	4	2.5	2700	1	300,000	310,000
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
home n	5	3.5	3600	3	450,000	450,000

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$X \approx C E$

$$10000 * \text{bathrooms} + 10 * (\text{sq. ft.}) \approx \text{list price}$$

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