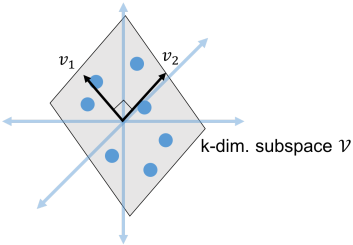
# COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 15

# LAST CLASS: EMBEDDING WITH ASSUMPTIONS

**Set Up:** Assume that data points $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$ lie in some $k$-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$.




Let $\vec{v}_1, \ldots, \vec{v}_k$ 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.

$$\|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2^2 = \|\vec{x}_i - \vec{x}_j\|_2^2.$$

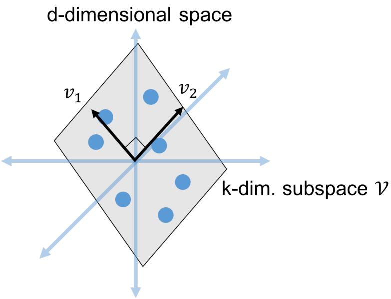
Letting $\tilde{x}_i = \mathbf{V}^T \vec{x}_i$, we have a perfect embedding from $\mathcal{V}$ into $\mathbb{R}^k$.

# LAST CLASS: PROJECTION VIEW

**Claim:** If $\vec{x}_1, \ldots, \vec{x}_n$ 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

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

- $\mathbf{V}\mathbf{V}^T$ is a projection matrix, which projects the rows of $\mathbf{X}$ (the data points $\vec{x}_1, \ldots, \vec{x}_n$) onto the subspace $\mathcal{V}$.




$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

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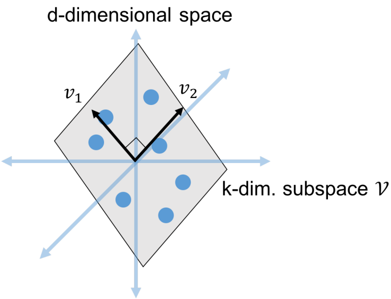


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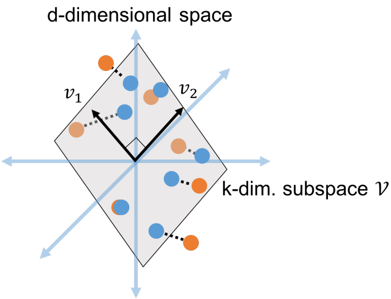


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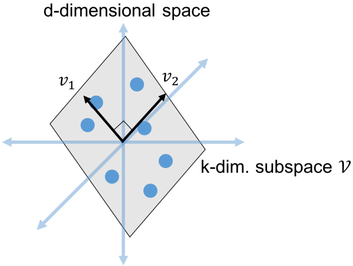
Assume that data points $\vec{x}_1, \ldots, \vec{x}_n$ lie close to any $k$-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$.



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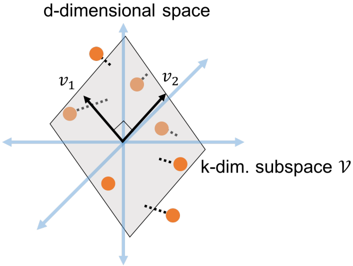


Will show above in homework. Today's focus: How do we find $\mathcal{V}$ and $\mathbf{V}$?

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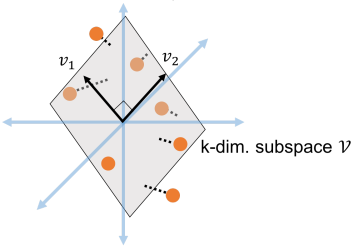


Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns, $\mathbf{V}^T \vec{x}_i \in \mathbb{R}^k$ is still a good embedding for $x_i \in \mathbb{R}^d$ and $\mathbf{XVV}^T$ is still a good approximation for $\mathbf{X}$:

$$\mathbf{XVV^T} = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2.$$

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# A STEP BACK: WHY LOW-RANK APPROXIMATION?

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

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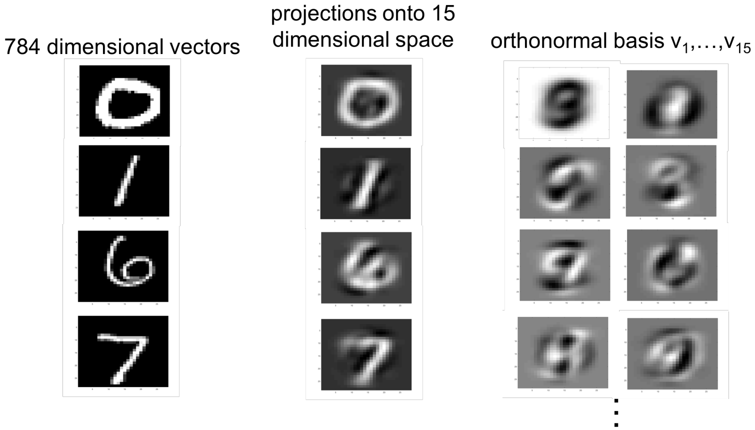

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| home 1 | 2 | 2 | 1800 | 2 | 200,000 | 195,000 |
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**Quick Exercise 1 :** Show that $\mathbf{V}\mathbf{V}^T$ is idempotent. I.e., $(\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T)\vec{y} = (\mathbf{V}\mathbf{V}^T)\vec{y}$ for any $\vec{y} \in \mathbb{R}^d$.

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**Quick Exercise 2:** The projection is orthogonal to its complement: For any $\vec{y} \in \mathbb{R}^d$, $\langle \mathbf{V}\mathbf{V}^T\vec{y}, (\mathbf{I} - \mathbf{V}\mathbf{V}^T)\vec{y} \rangle = 0$

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**Implies the Pythagorean Theorem:** Show that for any $\vec{y} \in \mathbb{R}^d$,

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

# BEST FIT SUBSPACE

If $\vec{x}_1, \ldots, \vec{x}_n$ are close to a $k$-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{X}\mathbf{V}\mathbf{V}^T$ and $\mathbf{X}\mathbf{V}$ gives optimal embedding of $\mathbf{X}$ in $\mathcal{V}$. How do we find $\mathcal{V}$ (equivalently $\mathbf{V}$)?

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\begin{aligned}
\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{XVV}^T\|_F^2 &= \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{XVV}^T)_{i,j})^2 \\
&= \sum_{i=1}^{n} \|\vec{x}_i - \mathbf{VV}^T \vec{x}_i\|_2^2 \\
&= \sum_{i=1}^{n} \|\vec{x}_i\|_2^2 - \|\mathbf{VV}^T \vec{x}_i\|_2^2
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\mathop{\arg\min}_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 &= \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_{i,j})^2 \\
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\end{aligned}$$

So want to maximize $\sum_i \|\mathbf{V}\mathbf{V}^T \vec{x}_i\|_2^2 = \sum_i \vec{x}_i^T \mathbf{V}\mathbf{V}^T\mathbf{V}\mathbf{V}^T \vec{x}_i = \sum_i \|\mathbf{V}^T \vec{x}_i\|_2^2$

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Surprisingly, can find the columns of $\mathbf{V}$, $\vec{v}_1, \ldots, \vec{v}_k$ greedily.

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These are exactly the top $k$ eigenvectors of $\mathbf{X}^T\mathbf{X}$.

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