COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2022.

Lecture 15

Logistics

- Midterms should be graded by end of the week.
- Will release grades once we are done and hand them back in class next week.
- Quiz due Monday 8pm as usual this week.

Summary

Last Few Classes:

The Johnson-Lindenstrauss Lemma

- Reduce n data points in any dimension d to $O\left(\frac{\log n/\delta}{\epsilon^2}\right)$ dimensions and preserve (with probability $\geq 1 - \delta$) all pairwise distances up to $1 \pm \epsilon$.
- Compression is linear via multiplication with a random, data oblivious, matrix (linear compression)

High-Dimensional Geometry

- Why high-dimensional space is so different than low-dimensional space.
- How the JL Lemma can still work, and why it is optimal.

Summary

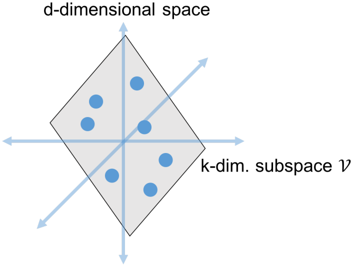
Next Few Classes: Low-rank approximation, the SVD, and principal component analysis (PCA).

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



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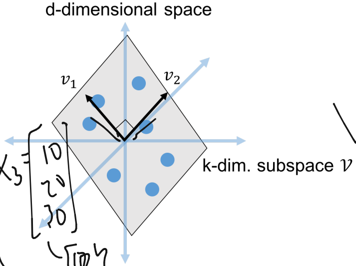

d = 3
k = 1

$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ → [1] $x_2 = \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}$ → [2] $x_3 = \begin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix}$ → [10]

$V = d\begin{bmatrix} | & | & & | \\ V_1 & V_2 & \cdots & V_k \\ | & | & & | \end{bmatrix}$ (k columns)

Claim: 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. For all $\vec{x}_i, \vec{x}_j$:

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

k×d d×1

k×1

$V^T x_i \in \mathbb{R}^k$

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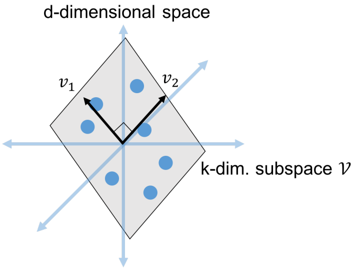

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$$\|\mathbf{V}^T\vec{x}_i - \mathbf{V}^T\vec{x}_j\|_2 = \|\vec{x}_i - \vec{x}_j\|_2.$$

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

Dot Product Transformation

Claim: 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. For all $\vec{x}_i, \vec{x}_j \in \mathcal{V}$:

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

$\exists c_i, c_j \in \mathbb{R}^k$: $x_i = Vc_i \quad x_j = Vc_j$

x_i is a linear comb. of $v_1 \ldots v_k$: $v_1 c_i(1) + v_2 c_i(2) \ldots v_k c_i(k)$

$$\|V^T V c_i - V^T V c_j\|_2 = \|Vc_i - Vc_j\|_2$$

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

$$\|c_i - c_j\|_2^2 = \|Vc_i - Vc_j\|_2^2$$ (want to prove)

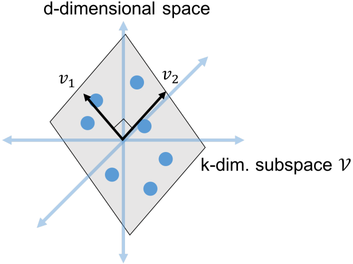
Fact: for any y, $\|y\|_2^2 = \langle y, y \rangle = y^T y = \sum_{i=1}^{d} y(i)\, y(i) = \sum y(i)^2 = \|y\|_2^2$

$$\|Vc_i - Vc_j\|_2^2 = \|V(c_i - c_j)\|_2^2 = (c_i - c_j)^T V^T V (c_i - c_j) = (c_i - c_j)^T (c_i - c_j) = \|c_i - c_j\|_2^2$$

$[V(c_i - c_j)]^T$

Embedding with Assumptions

Main Focus of Upcoming Classes: 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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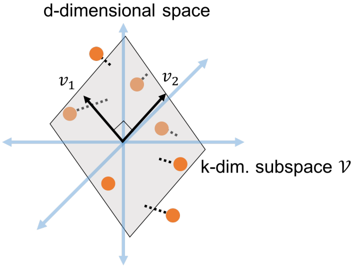

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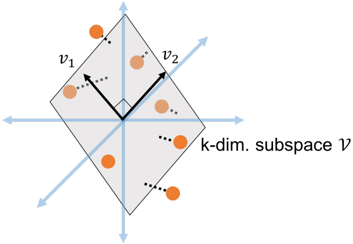

Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns, $\mathbf{V}^T\vec{x}_i \in \mathbb{R}^k$ is still a good embedding for $x_i \in \mathbb{R}^d$.

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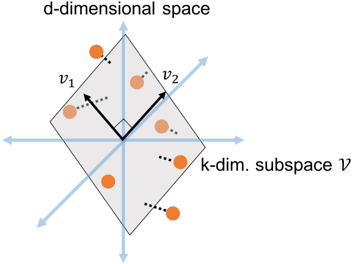

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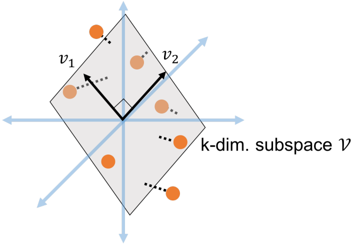

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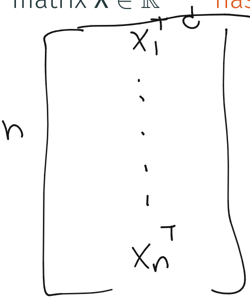
- How do we find $\mathcal{V}$ and $\mathbf{V}$?
- How good is the embedding?

Low-Rank Factorization

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



(dim of col(X)
dim of row(X)
max # linearly ind. rows/columns

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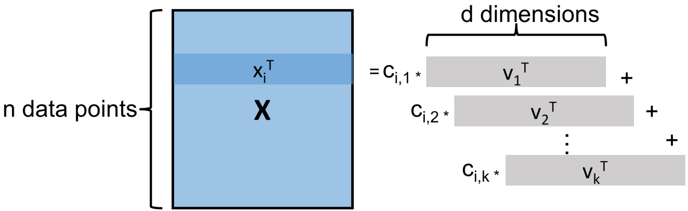
- Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$, can write $\vec{x}_i$ as:

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



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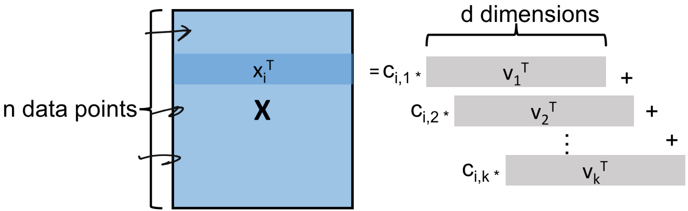
- So $\vec{v}_1, \ldots, \vec{v}_k$ span the rows of $\mathbf{X}$ and thus $\mathbf{rank}(\mathbf{X}) \leq k$.



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- Every data point $\vec{x}_i$ (row of $\mathbf{X}$) can be written as $\vec{x}_i = \mathbf{V}\vec{c}_i = c_{i,1} \cdot \vec{v}_1 + \ldots + c_{i,k} \cdot \vec{v}_k$.

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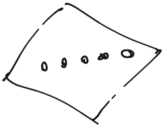

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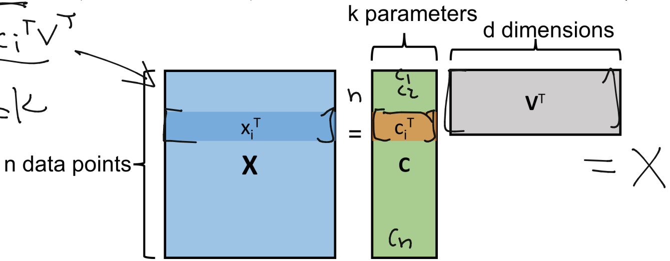
$x_i^T = c_i^T V^T$

rank(X) ≤ k



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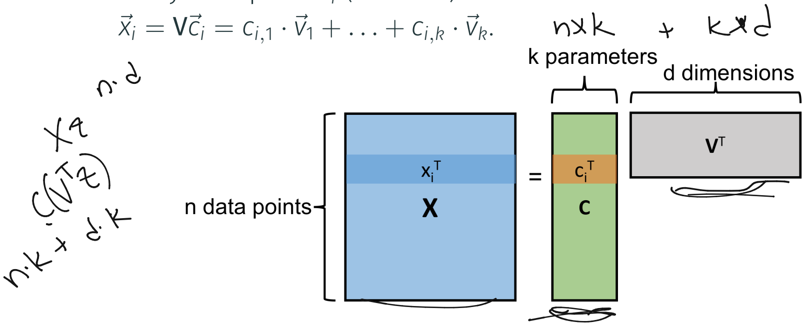

- $\mathbf{X}$ can be represented by $(n + d) \cdot k$ parameters vs. $n \cdot d$.

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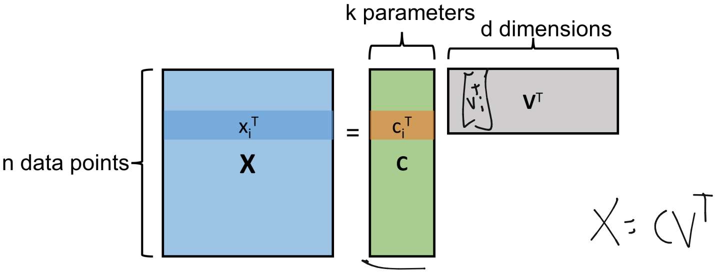

- $\mathbf{X}$ can be represented by $(n + d) \cdot k$ parameters vs. $n \cdot d$.
- The rows of $\mathbf{X}$ are spanned by k vectors: the columns of $\mathbf{V}$ $\implies$ the columns of $\mathbf{X}$ are spanned by k vectors: the columns of $\mathbf{C}$.

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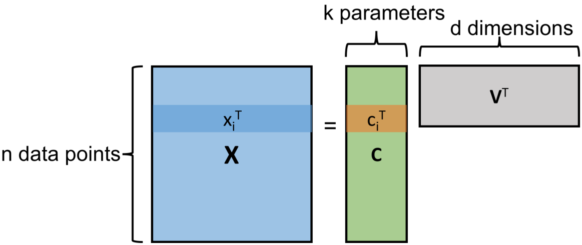
Low-Rank Factorization

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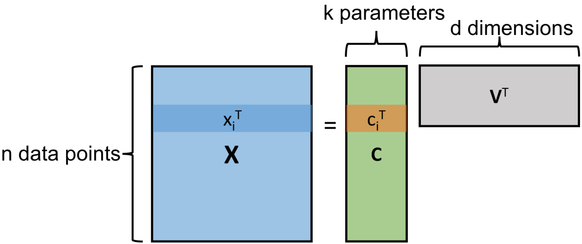

Exercise: What is this coefficient matrix $\mathbf{C}$? **Hint:** Use that $\mathbf{V}^T\mathbf{V} = \mathbf{I}$.

$XV = CV^TV \Rightarrow XV = C$

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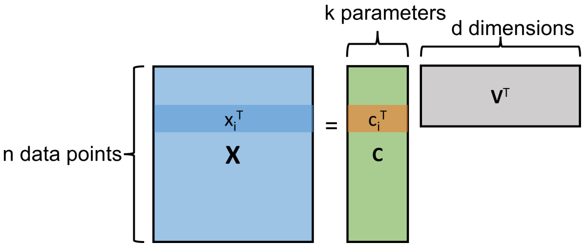

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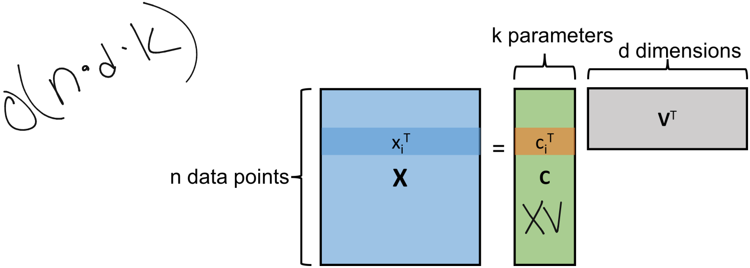

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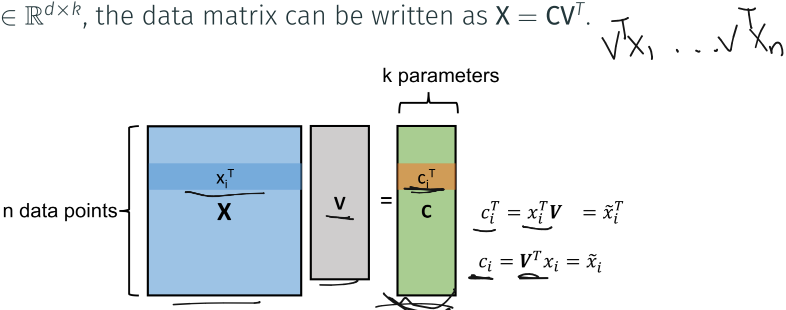

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Projection View

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XV

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n×d d×k k×d = n×d

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

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$V^T V = I$

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- $\mathbf{V}\mathbf{V}^T$ is a projection matrix, which projects vectors onto the subspace $\mathcal{V}$.

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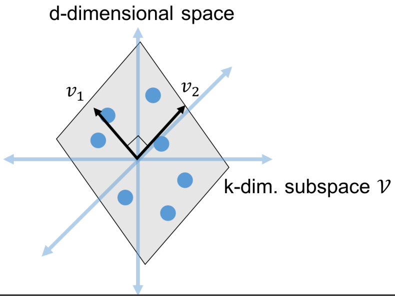

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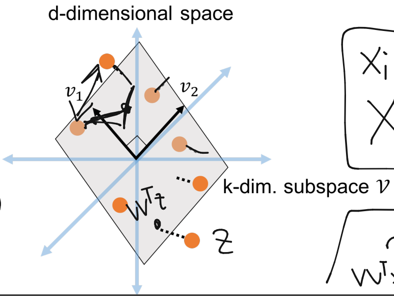

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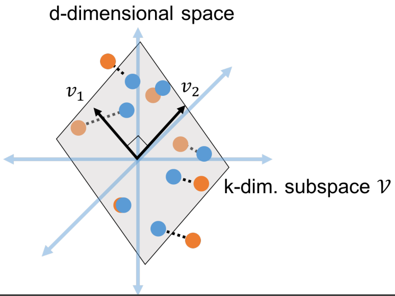

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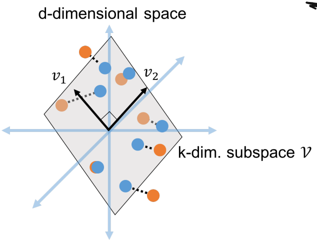

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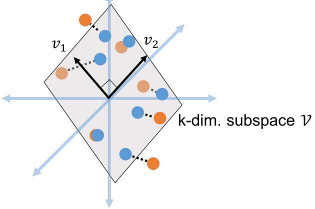

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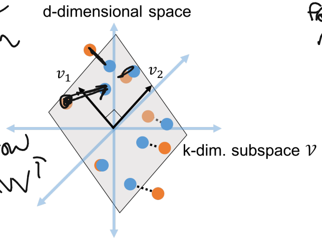

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$$\mathbf{X}\mathbf{V}\mathbf{V}^T = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - \mathbf{B}_{i,j})^2.$$

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$\|X - XVV^T\|_F^2$

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

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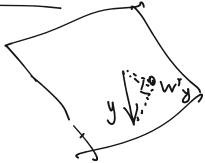
Properties of Projection Matrices

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:

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



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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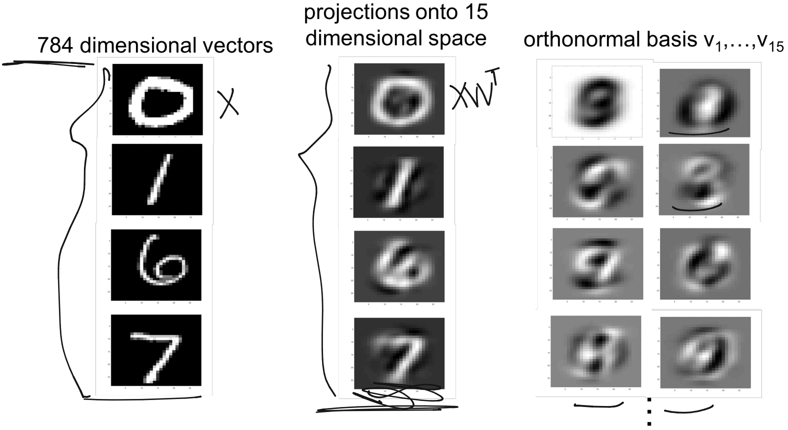

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