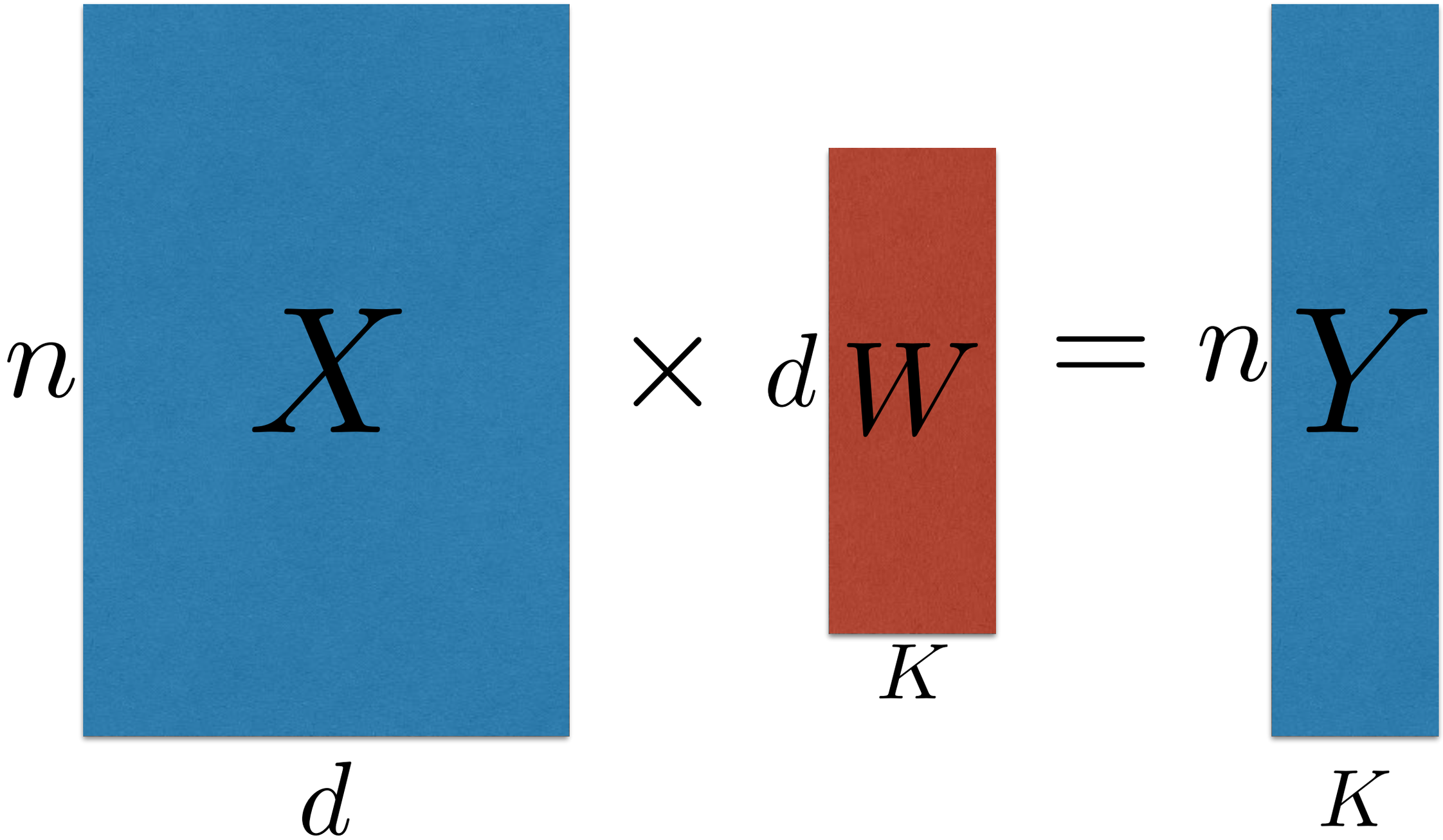
Machine Learning for Data Science (CS4786)
Lecture 4

PCA and Random Projections

Dim Reduction: Linear Transformation



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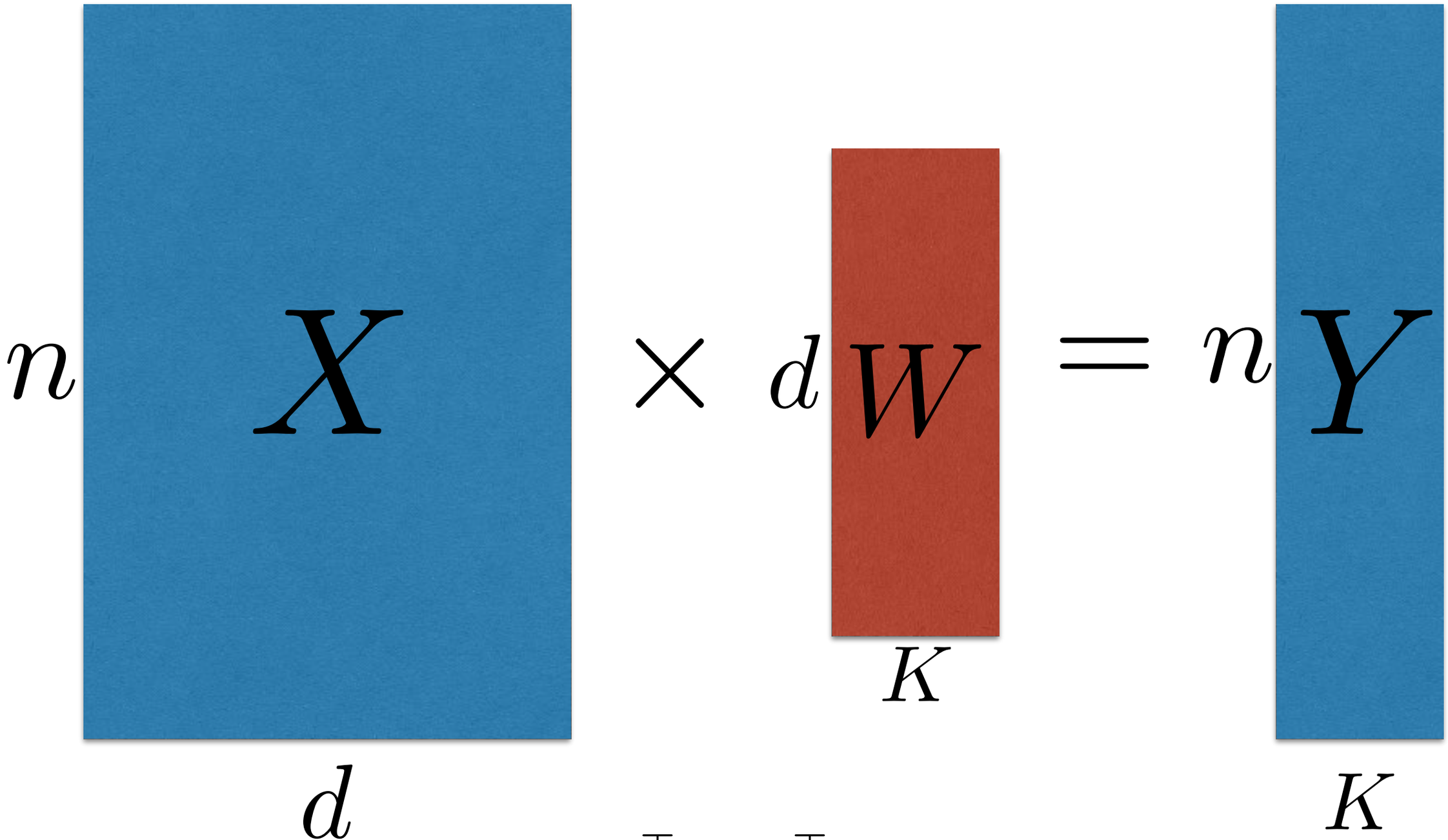


$$\mathbf{y}_i^\top = \mathbf{x}_i^\top W$$

PCA: Variance Maximization

- Pick directions along which data varies the most

$$\text{Spread} = \frac{1}{n}\sum_{t=1}^{n} \text{dist}^2 \left(y_t, \frac{1}{n}\sum_{t=1}^{n} y_t \right) = \sum_{j=1}^{K} \mathbf{w}_j^\top \Sigma \mathbf{w}_j$$

$$\text{Maximize} \sum_{j=1}^{K} \mathbf{w}_j^\top \Sigma \mathbf{w}_j$$

$$\text{s.t. } \forall j, \|\mathbf{w}_j\|_2^2 = 1 \;\&\; \mathbf{w}_j \perp \mathbf{w}_i$$

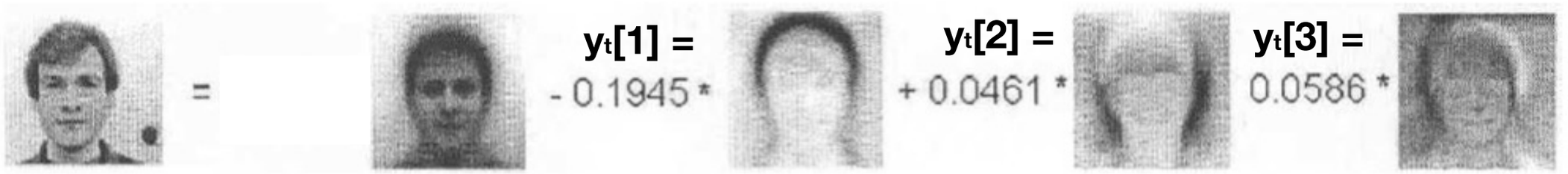
Σ is the covariance matrix

This solutions is given by W = Top K eigenvectors of Σ

Principal Component Analysis (PCA)

Turk & Pentland'91

Eigen Face:



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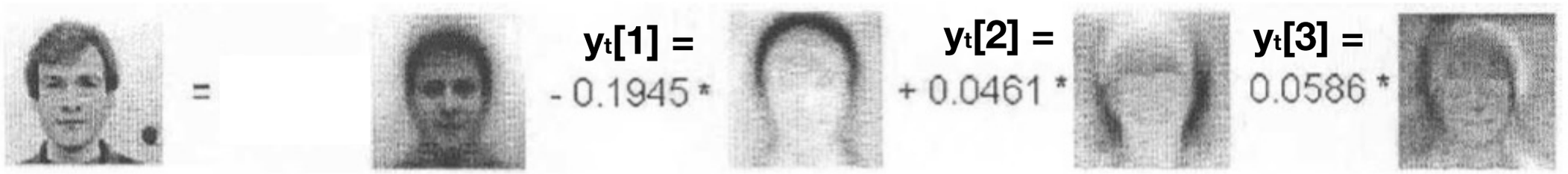

- Each x_t (each row of X) is a face image (vectorized version)

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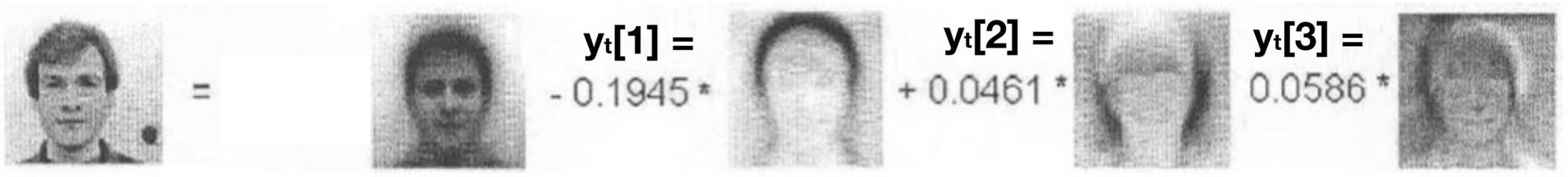

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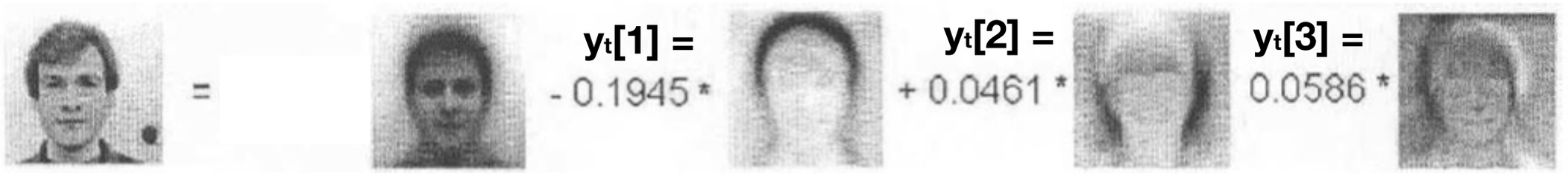

- Each x_t (each row of X) is a face image (vectorized version)
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- w_i's are orthogonal to each other and of unit length

PCA: Minimizing Reconstruction Error

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where $\mathbf{w}_1, \ldots, \mathbf{w}_d \in \mathbb{R}^d$ are the orthonormal basis and $\mu = \frac{1}{n}\sum_{t=1}^{n} x_t$.

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- Represent data as linear combination of just K orthonormal basis,

$$\hat{\mathbf{x}}_t = \mu + \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j$$

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$$= \sum_{j=k+1}^{d} \mathbf{y}_t[j]^2 \|\mathbf{w}_j\|_2^2 \quad (\text{last step because } \mathbf{w}_j \perp \mathbf{w}_i)$$

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$$\text{Take K} = 0 \text{ so that } \hat{\mathbf{x}}_t = \mu$$

Maximize Total Spread = Minimize Reconstruction Error

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Principal Component Analysis

1. $$\Sigma = \mathrm{cov}\left(X\right)$$

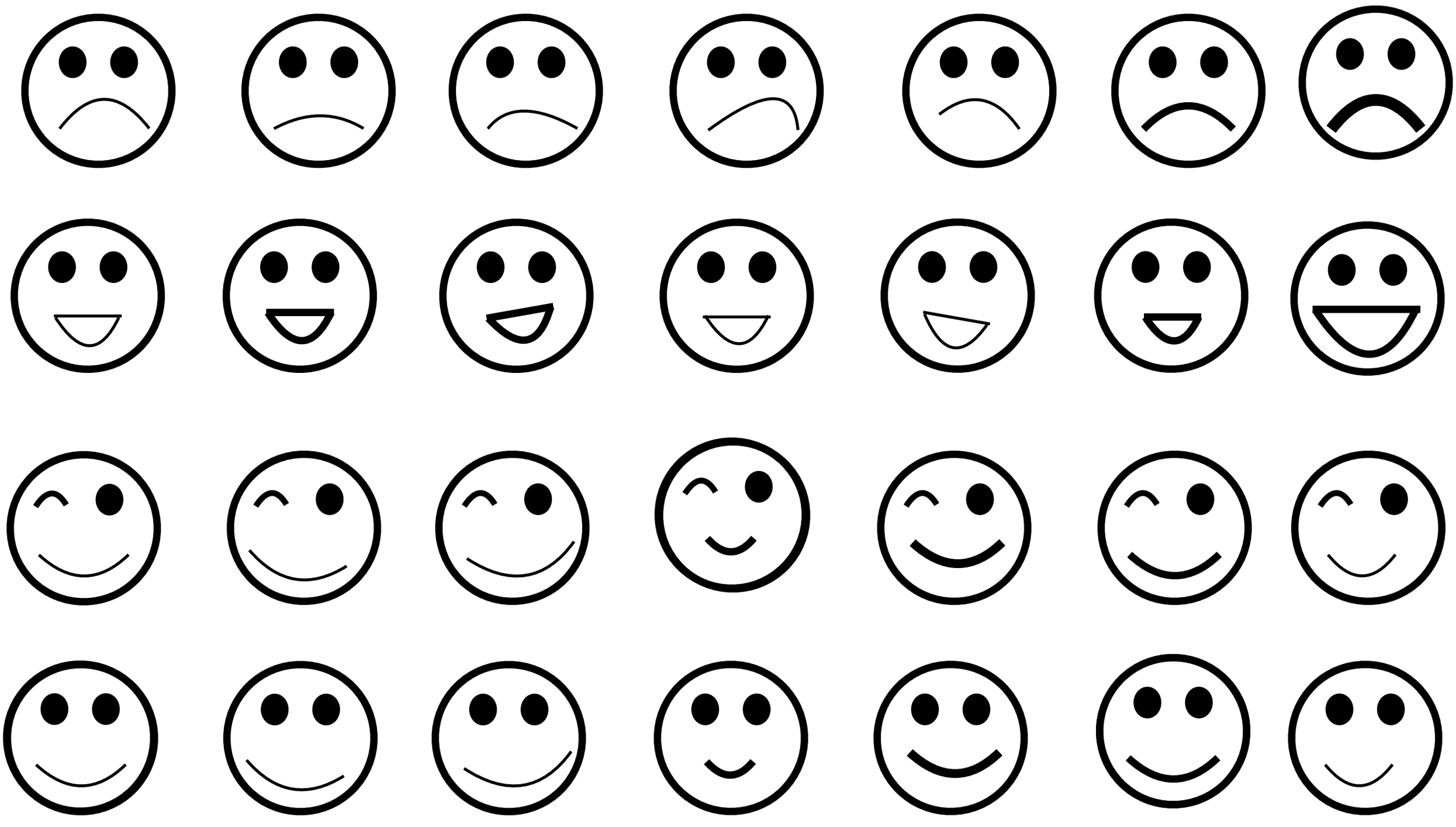
2. $$W = \mathrm{eigs}\left(\Sigma, K\right)$$

3. $$Y = X - \mu \times W$$

Reconstruction

4. $\hat{X} = Y \times W^{\top} + \mu$

Principal Component Analysis: Demo



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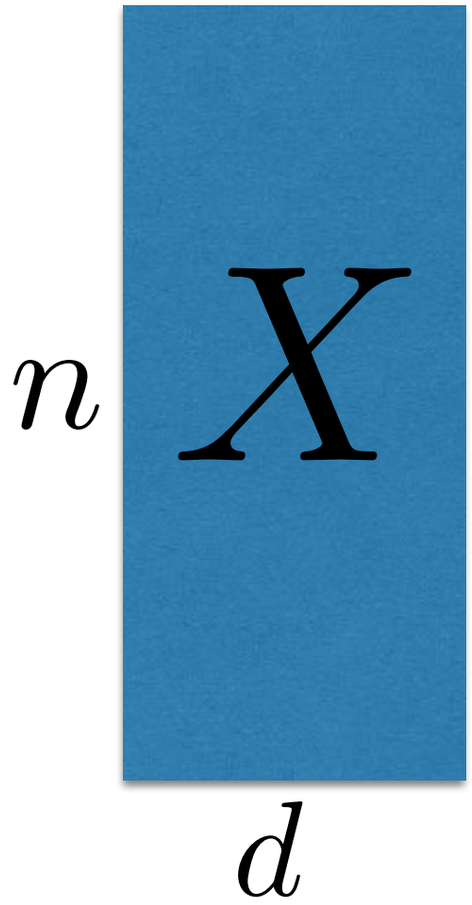
- Hence, matrix V is the same as matrix W got from eigen decomposition of Σ, eigenvalues are diagonal elements of D^2
- Alternative algorithm:

$$[U, V] = \text{SVD}(X - \mu, K) \quad W = V$$

The Tall, the Fat and the Ugly



The Tall, the Fat and the Ugly

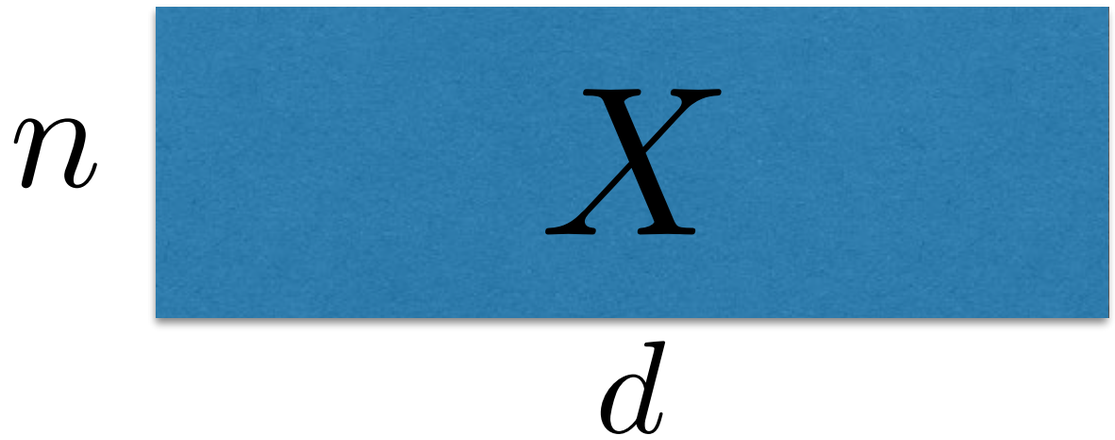
$$\underset{d}{\boxed{X^\top}}\underset{n}{\boxed{}} \times \underset{n}{\boxed{X}}\underset{d}{\boxed{}} \Big/ n = \underset{d}{\boxed{\Sigma}}\underset{d}{\boxed{}}$$

The Tall, the Fat and the Ugly

$$\underset{d}{\square}\underset{n}{\square^\top} \times \underset{n}{\square}\underset{d}{\square} \Big/ n = \underset{d}{\square}$$

$$\underset{d}{\square}\underset{K}{\square} = \text{Eigs}\left(\square, K\right)$$

The Tall, **the Fat** and the Ugly



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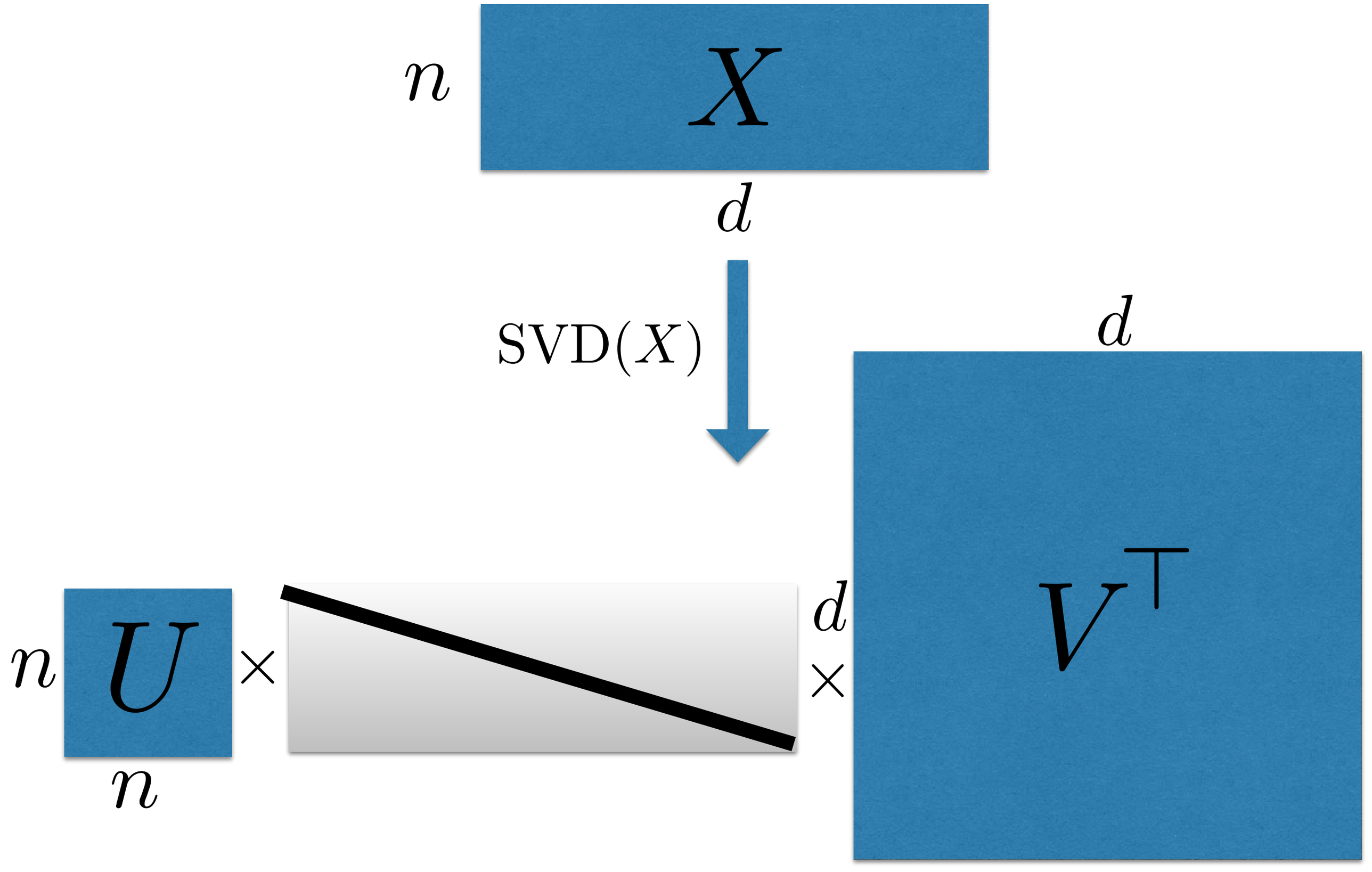

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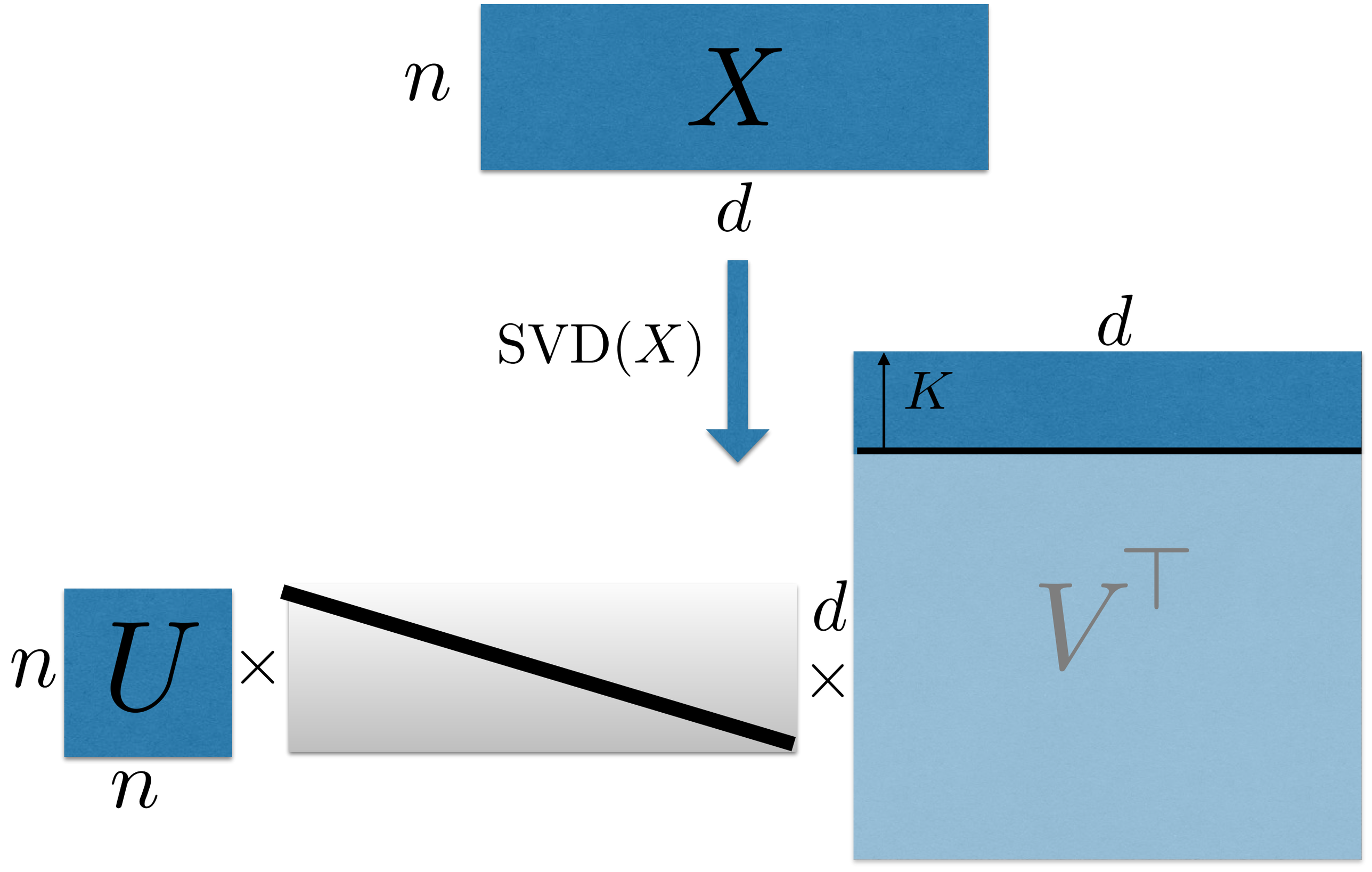

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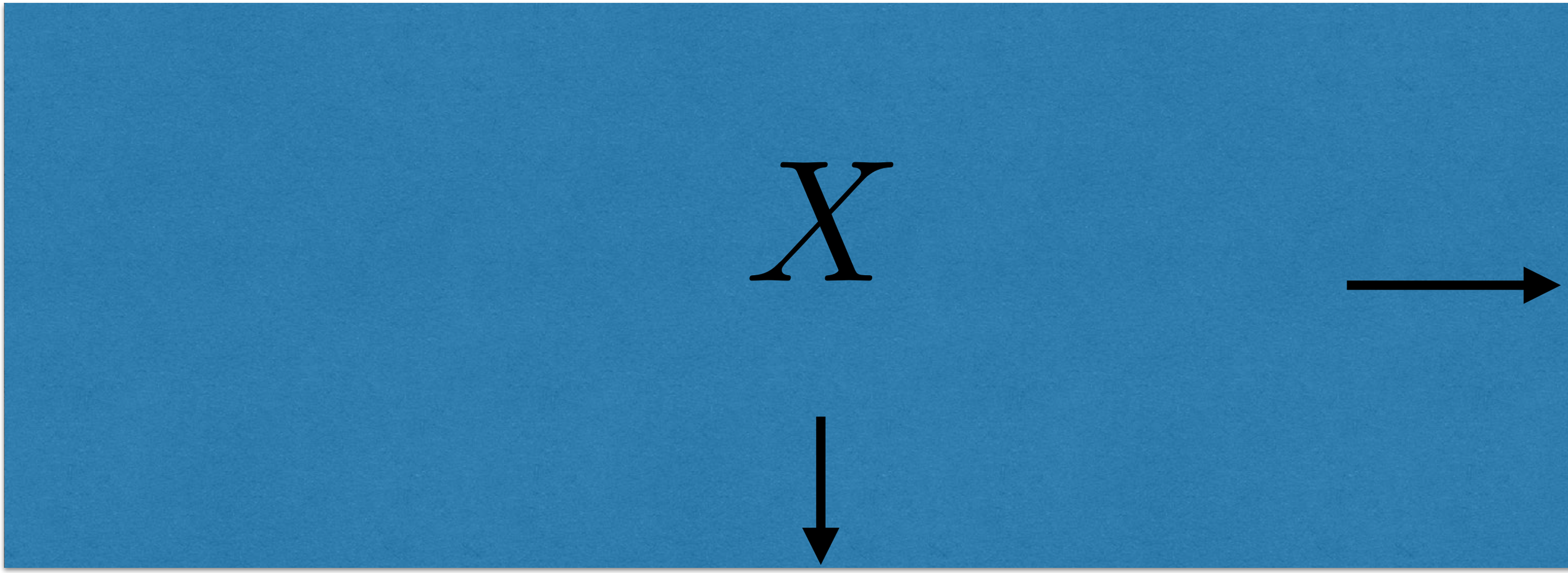

- d and n so large we can't even store in memory
- Only have time to be linear in $\text{size}(X) = n \times d$

I there any hope?

Pick a Random W

Pick a Random W

$$Y = X \times \begin{bmatrix} +1 & \dots & -1 \\ -1 & \dots & +1 \\ +1 & \dots & -1 \\ & \vdots & \\ +1 & \dots & -1 \end{bmatrix}_K \Big/ \sqrt{d}$$

Why should Random Projections even work?!

Random Projection

- What does “it works” even mean?

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  Distances between all pairs of data-points in low dim. projection is roughly the same as their distances in the high dim. space.

Random Projection

- What does "it works" even mean?

  Distances between all pairs of data-points in low dim. projection is roughly the same as their distances in the high dim. space.

That is, when K is "large enough", with "high probability", for all pairs of data points $i, j \in \{1, \ldots, n\}$,

$$(1-\epsilon)\left\|\mathbf{y}_i - \mathbf{y}_j\right\|_2 \leq \left\|\mathbf{x}_i - \mathbf{x}_j\right\|_2 \leq (1+\epsilon)\left\|\mathbf{y}_i - \mathbf{y}_j\right\|_2$$

WHY SHOULD RANDOM PROJECTIONS EVEN WORK?!

- Lets start with a one dimensional projection (K = 1)

$$y_t = \mathbf{x}_t^\top \mathbf{u} \quad \text{where each } \mathbf{u}[i] = \text{ random} \pm 1$$

- What is the expected value of:

1. $y_t - y_s$?
2. $(y_t - y_s)^2$?

Why should Random Projections even work?!

Hence for any $s, t \in \{1, \ldots, n\}$,

$$\mathbb{E}\left[|\mathbf{y}_s - \mathbf{y}_t|^2\right] = \|\mathbf{x}_s - \mathbf{x}_t\|_2^2$$

Lets try ...

Why should Random Projections even work?!

Hence for any $s, t \in \{1, \ldots, n\}$,

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Lets try ...

Law of large numbers says that average over multiple draws is close to expectation

WHY SHOULD RANDOM PROJECTIONS EVEN WORK?!

- Like repeating the experiment K times and averaging

$$\mathbf{y}_t[k] = \mathbf{x}_t^\top \mathbf{u}_k / \sqrt{K} \quad \text{where each } \mathbf{u}_k[i] = \text{ random} \pm 1$$

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This is an average over K trials

Pick a Random W

Pick a Random W

$$Y = X \times \begin{bmatrix} +1 & \dots & -1 \\ -1 & \dots & +1 \\ +1 & \dots & -1 \\ & \vdots & \\ +1 & \dots & -1 \end{bmatrix}_K \Big/ \sqrt{d}$$

Why should Random Projections even work?!

For any $\epsilon > 0$, if $K \approx \log(n/\delta)/\epsilon^2$, with probability $1 - \delta$ over draw of W, for all pairs of data points $i, j \in \{1, \ldots, n\}$,

$$(1-\epsilon)\left\|\mathbf{y}_i - \mathbf{y}_j\right\|_2^2 \leq \left\|\mathbf{x}_i - \mathbf{x}_j\right\|_2 \leq (1+\epsilon)\left\|\mathbf{y}_i - \mathbf{y}_j\right\|_2^2$$

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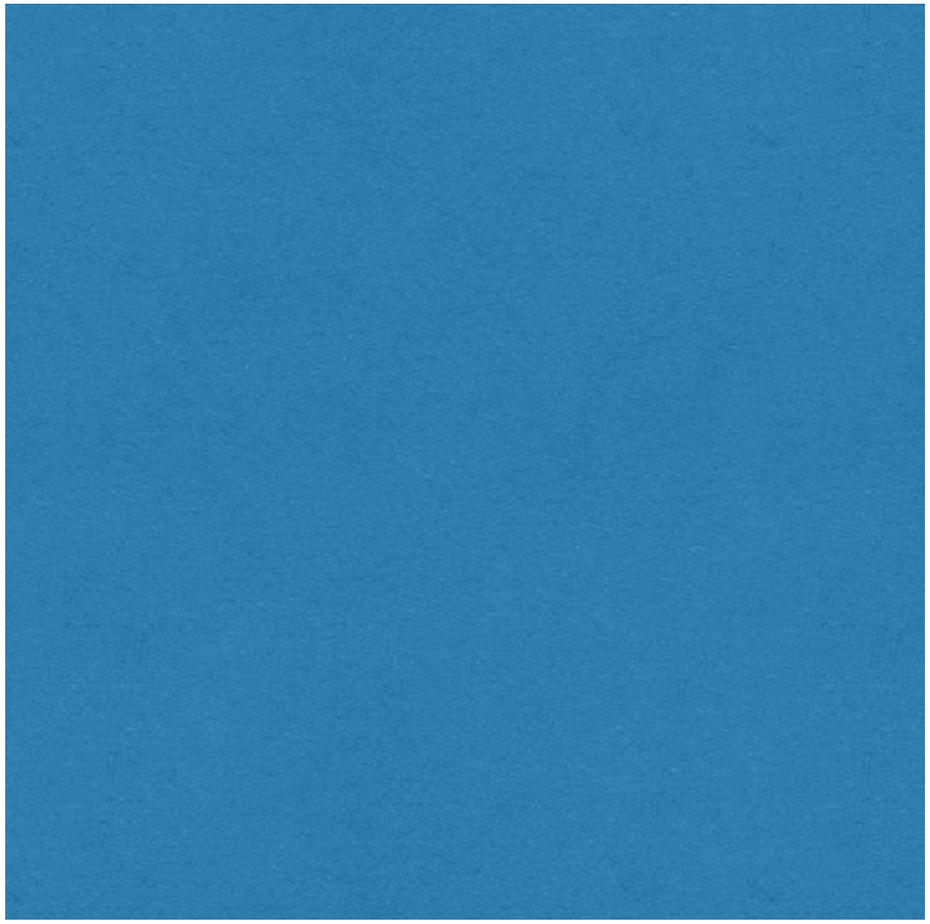
This is called the Johnson-Lindenstrauss lemma or JL lemma for short.

Why is this so Ridiculously Magical?

n=
1000



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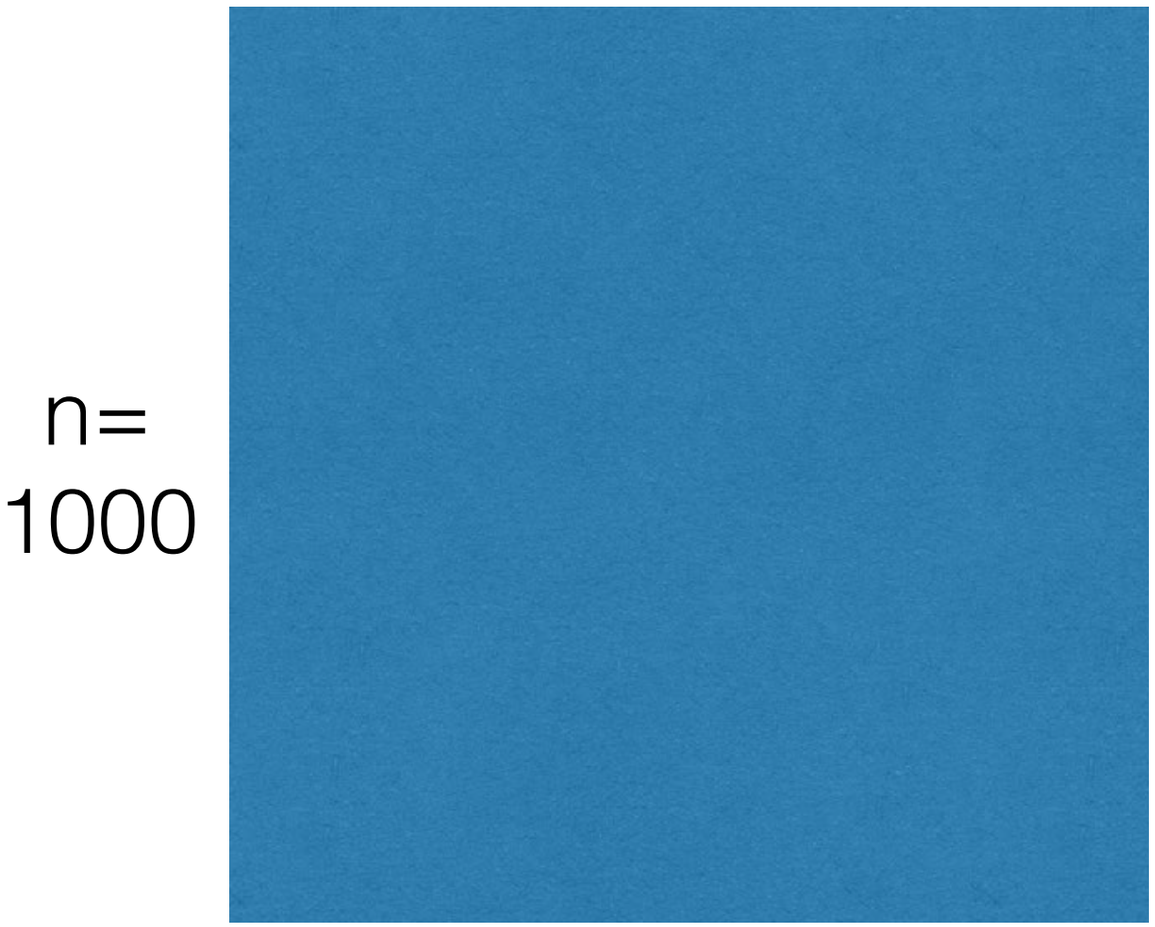

If we take $K = 69.1/\epsilon^2$, with probability 0.99 distances are preserved to accuracy ϵ

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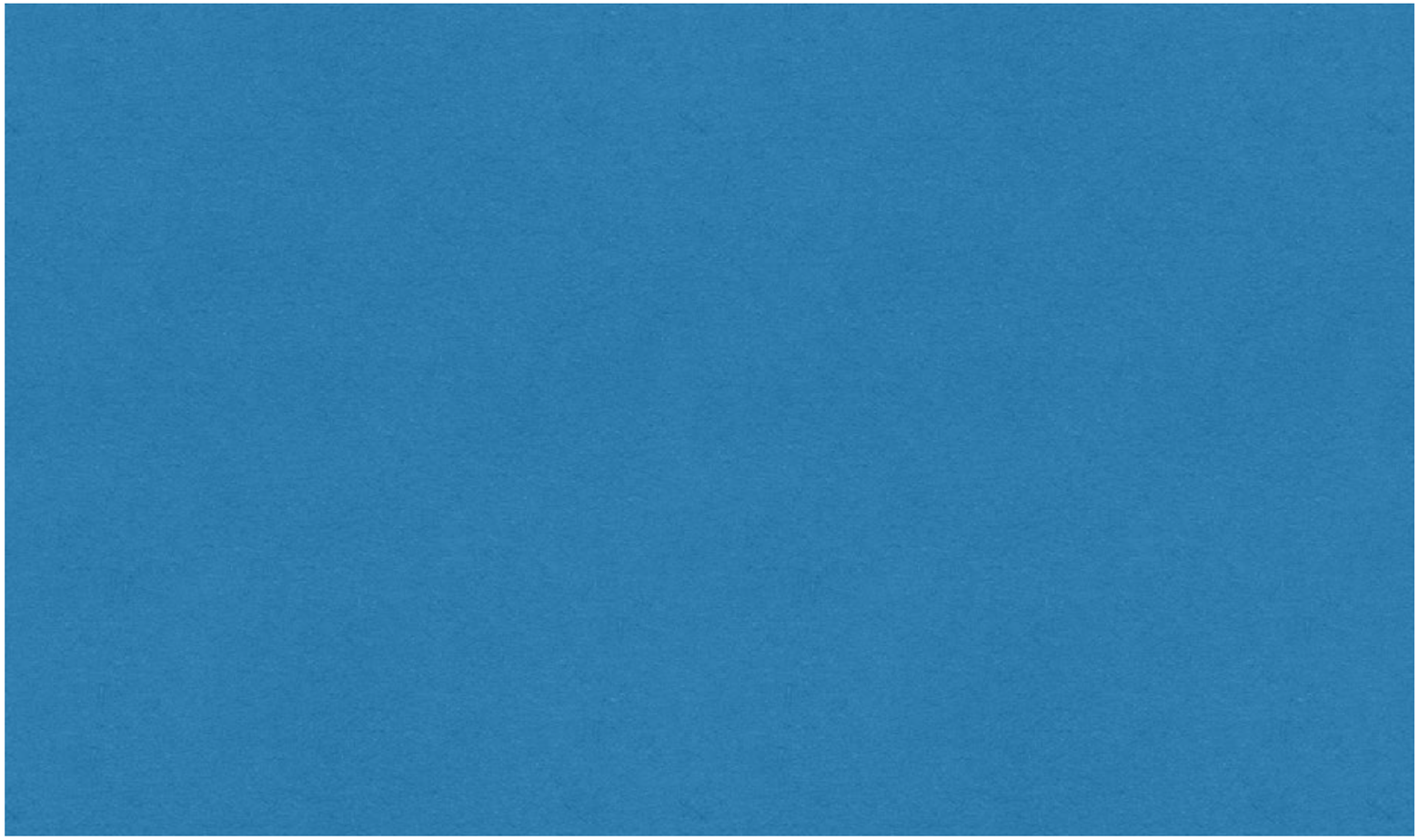

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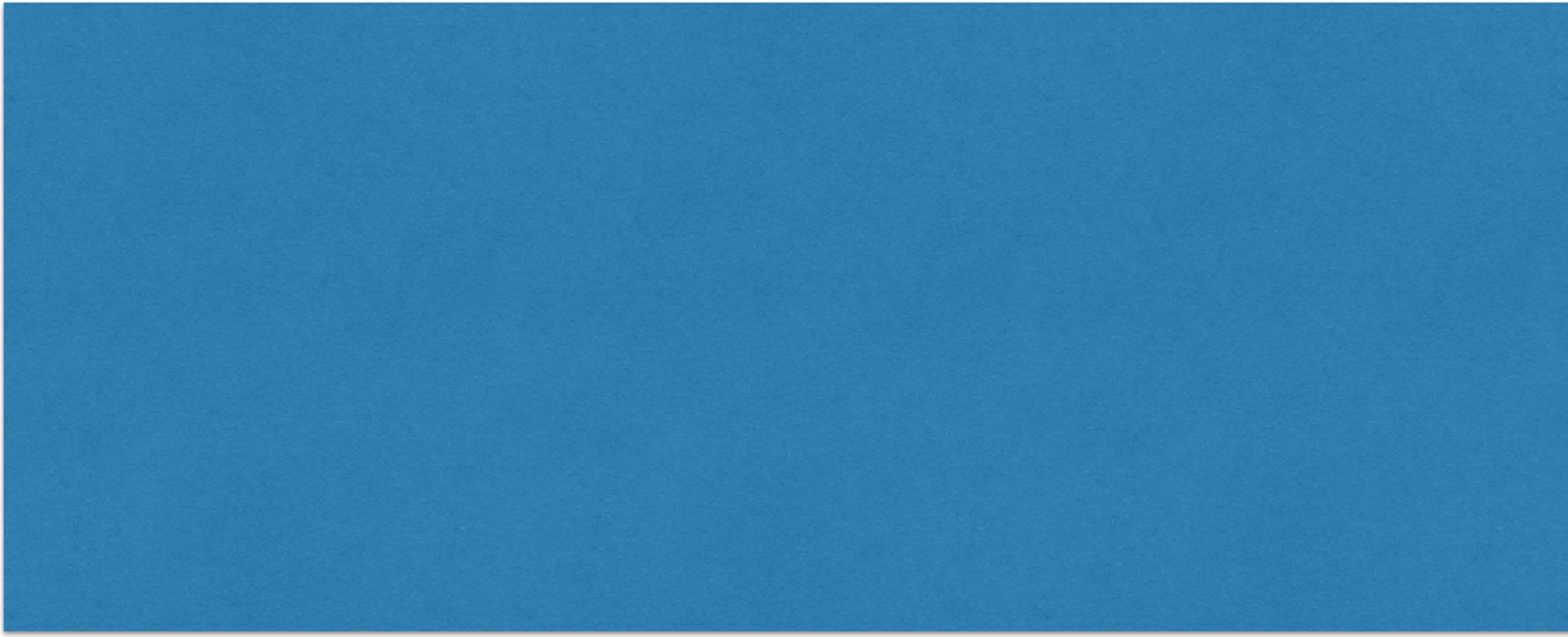

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