Machine Learning for Data Science (CS4786) Lecture 2

Dimensionality Reduction
&
Principal Component Analysis

Course Webpage :
http://www.cs.cornell.edu/Courses/cs4786/2016sp/

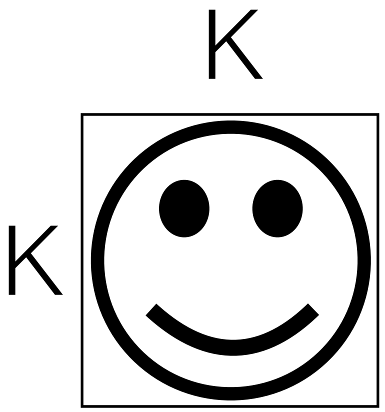
Announcements

- Diagnostic assignment due on 4th Feb (Thursday) beginning of class
- Course webpage is the official source of all class related information
- You will be added to CMS once you return Assignment 0 with your net-id on it.

Representing Data as Feature Vectors

- How do we represent data?
- Each data-point often represented as vector referred to as feature vector
- Eg. text document represented by vector in which each coordinate represents a word and value represents number of times the word occurred in the document
- Eg. Image represented as a vector where each coordinate represents a pixel and value represents the grayscale value of that pixel

Example: Images



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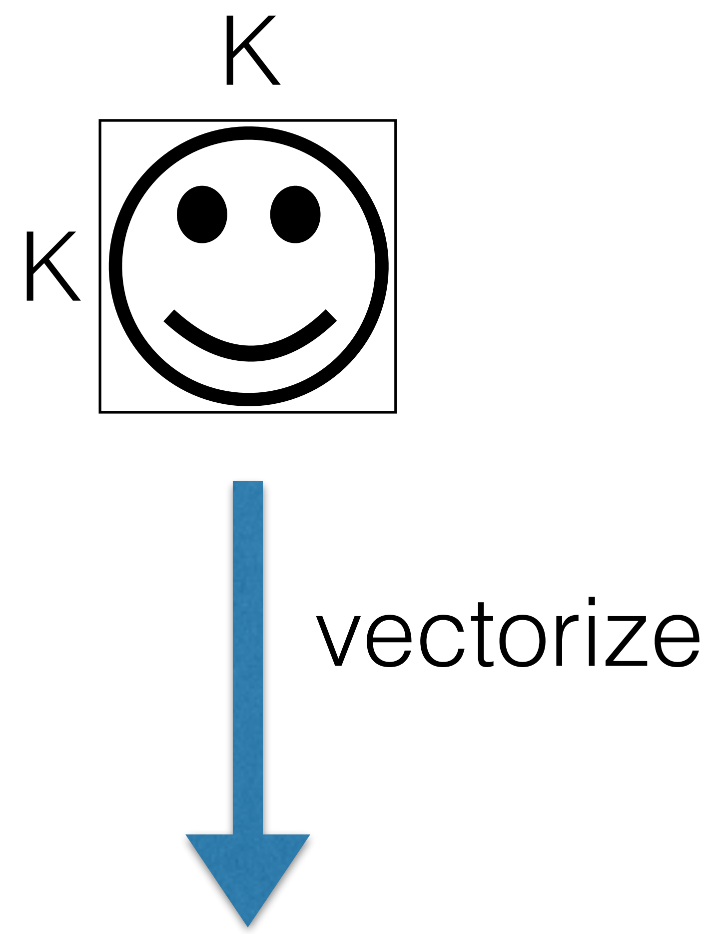
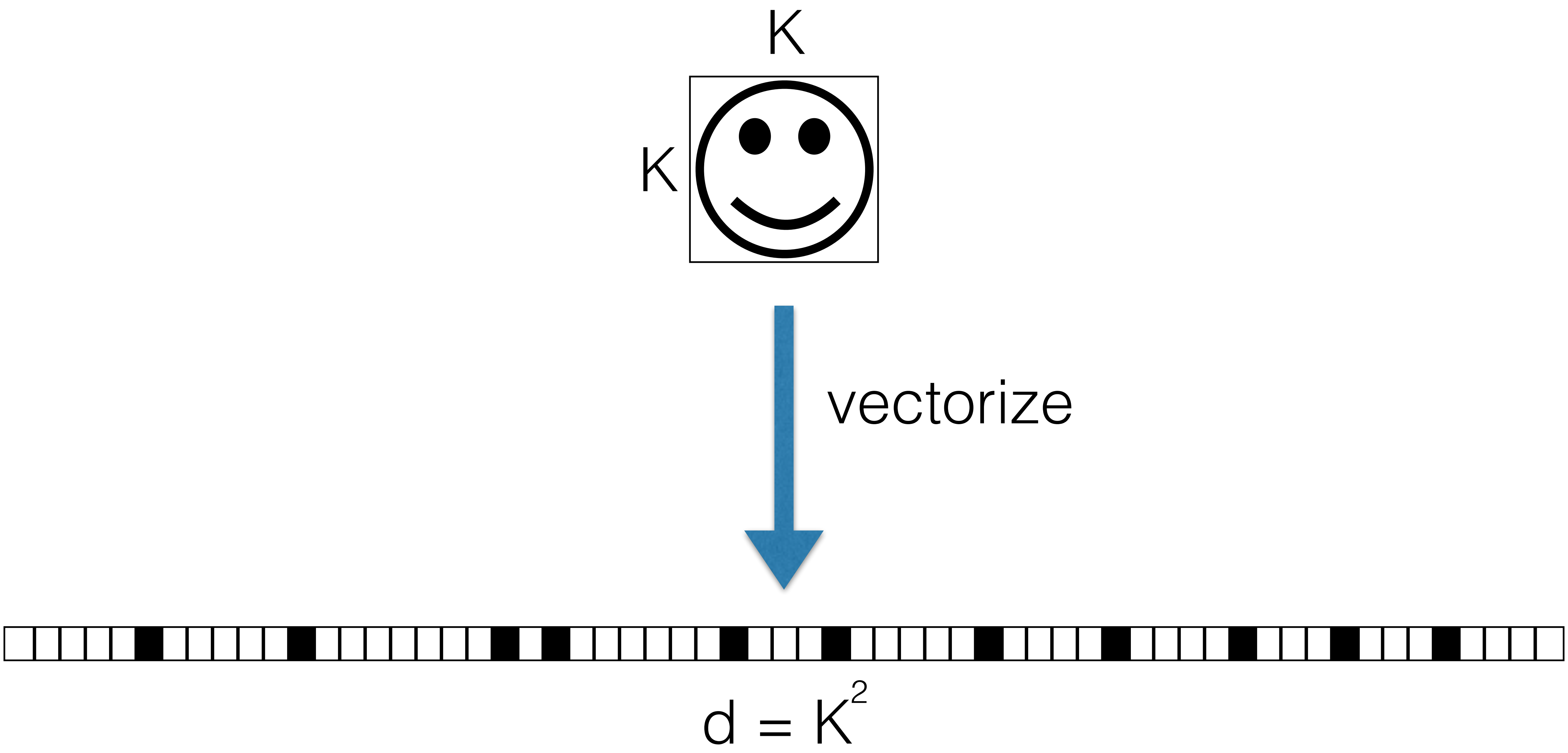


EXAMPLE: IMAGES



Example: Text (Bag of Words)

Documents:

car
engine
hood
tires
truck
trunk

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emissions
hood
make
model
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Chomsky
corpus
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car	Chomsky	corpus	emissions	engine	hood	make	model	noun	parsing	tagging	tires	truck	trunk	wonderful
1	0	0	0	1	1	0	0	0	0	0	1	1	1	0
1	0	0	1	0	1	1	1	0	0	0	0	0	1	0
0	1	1	0	0	0	0	0	1	1	1	0	0	0	1

Dimensionality Reduction

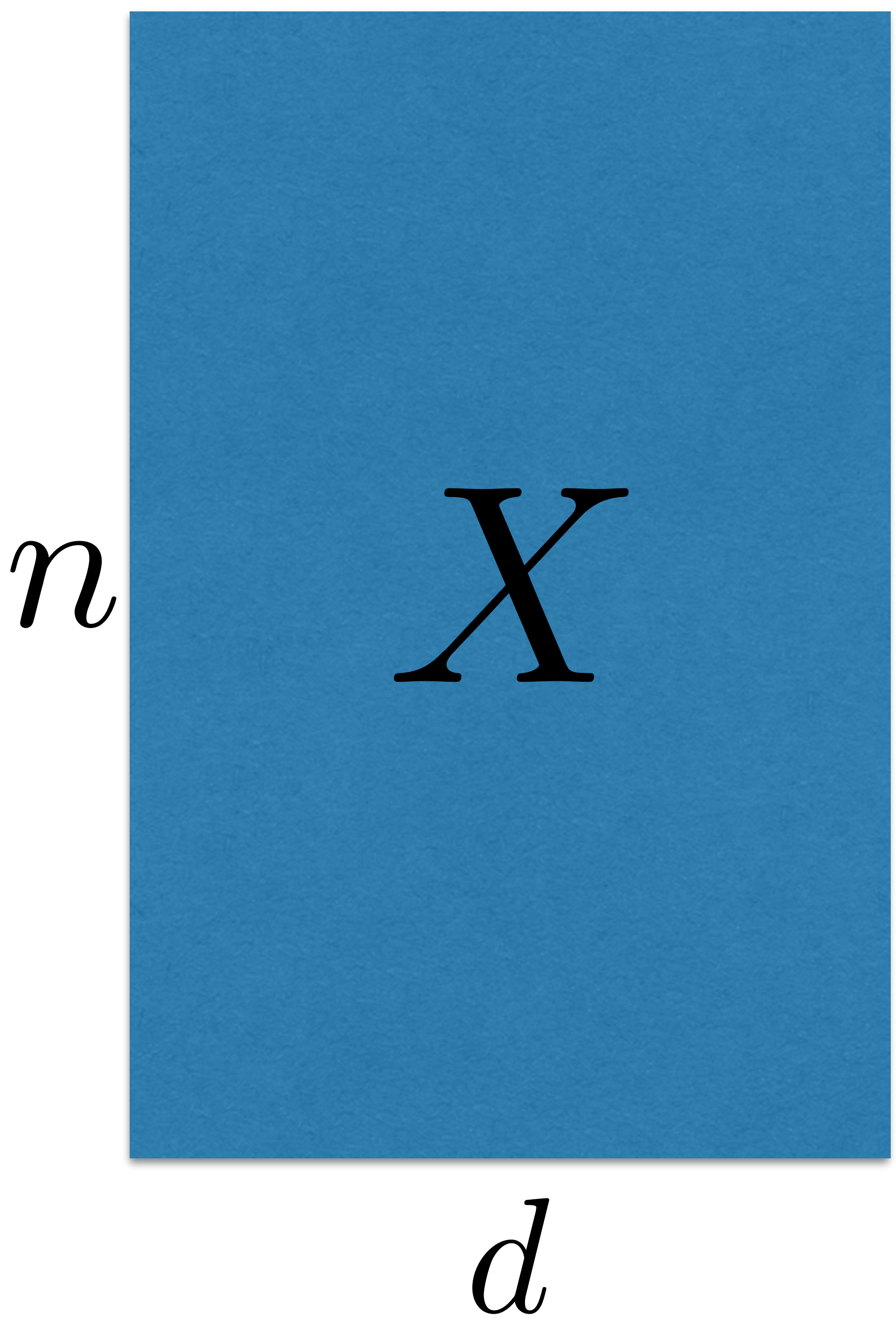
- You are provided with n data points each in $\mathbb{R}^d$
- Goal: Compress data into n, points in $\mathbb{R}^K$ where $K << d$
  - Retain as much information about the original data set
  - Retain desired properties of the original data set

Dimensionality Reduction

Given feature vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, compress the data points into low dimensional representation $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^K$ where $K << d$

Dimensionality Reduction

Dimensionality Reduction



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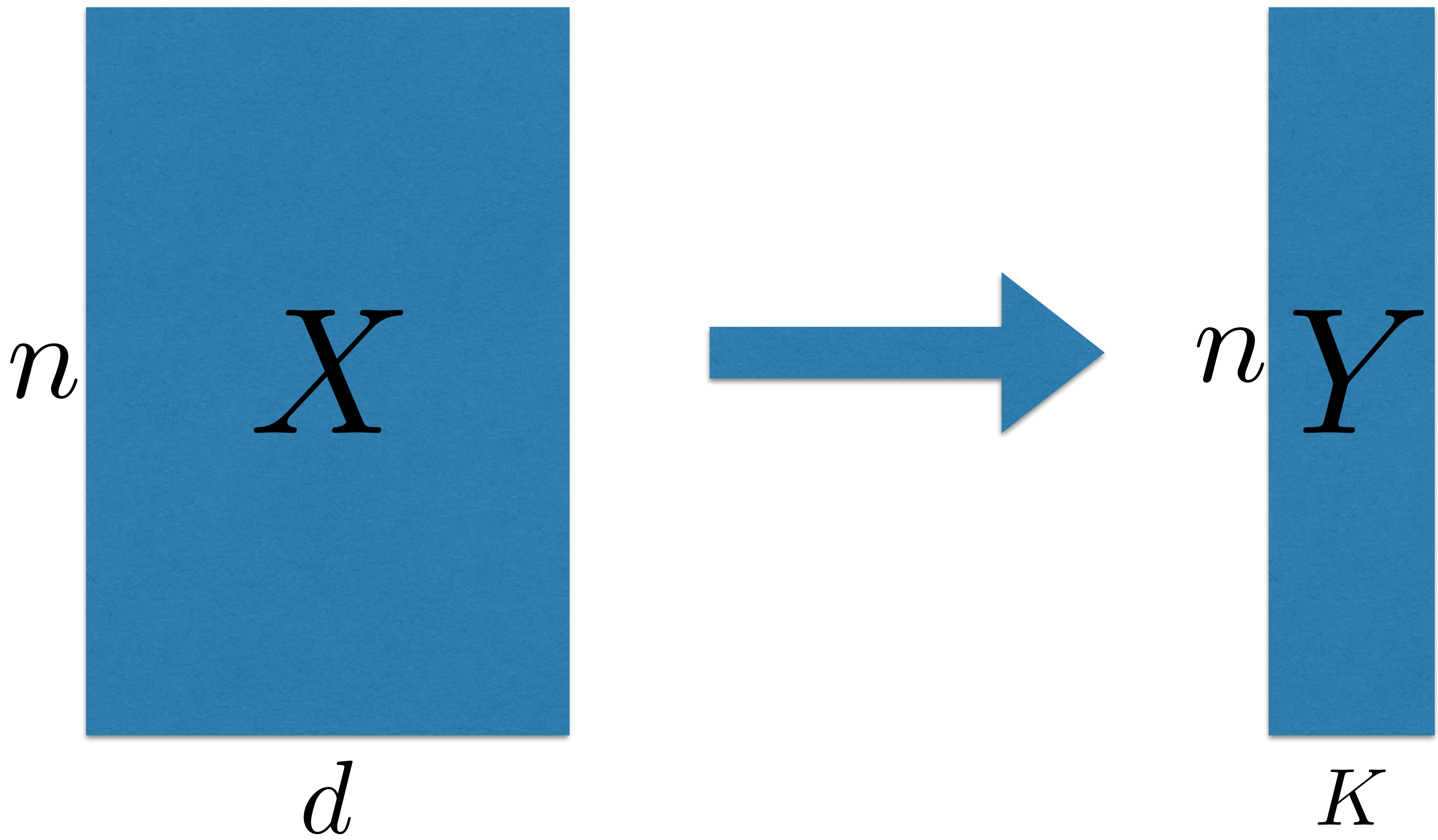
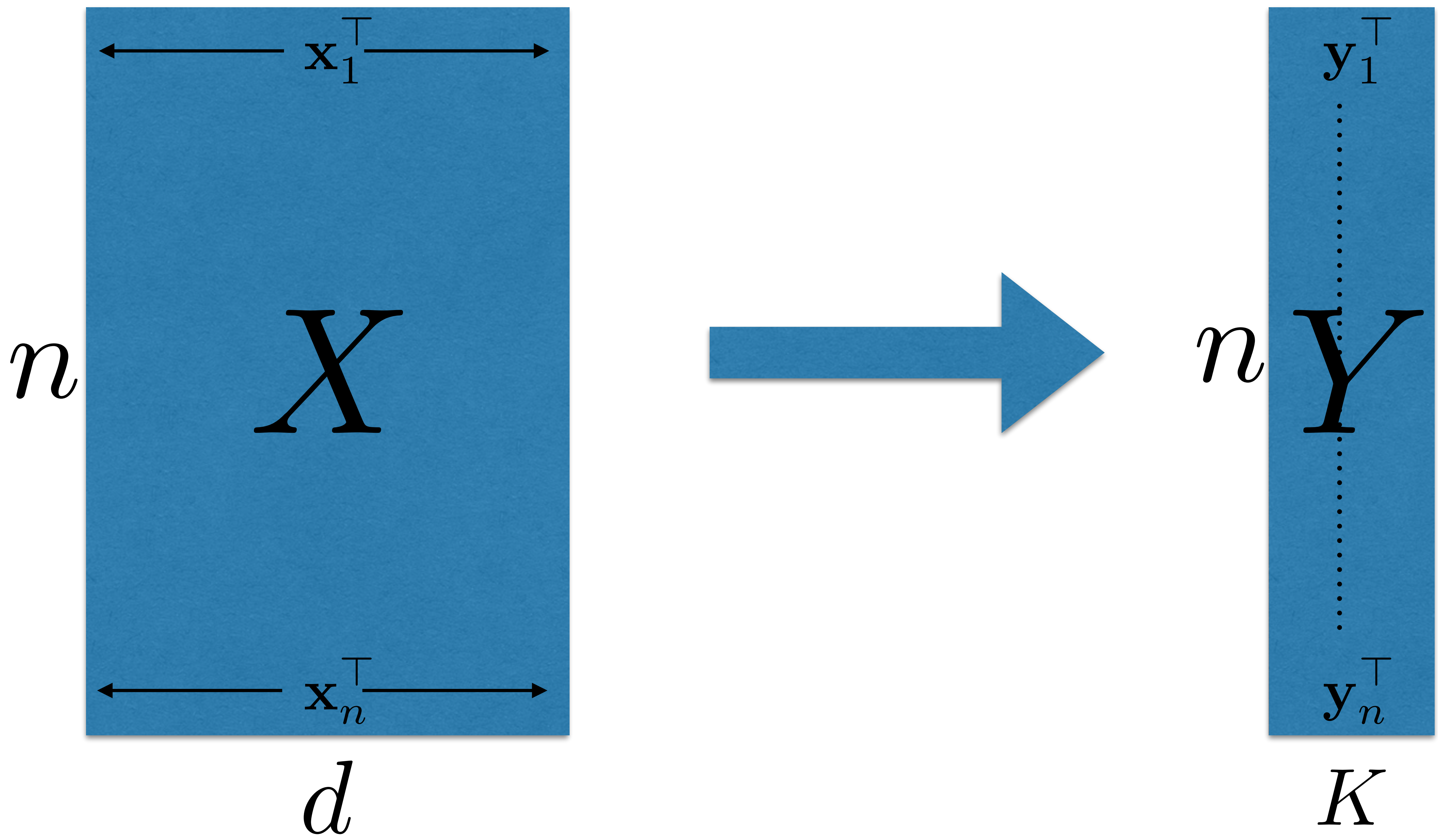


Dimensionality Reduction



Dimensionality Reduction

Desired properties:

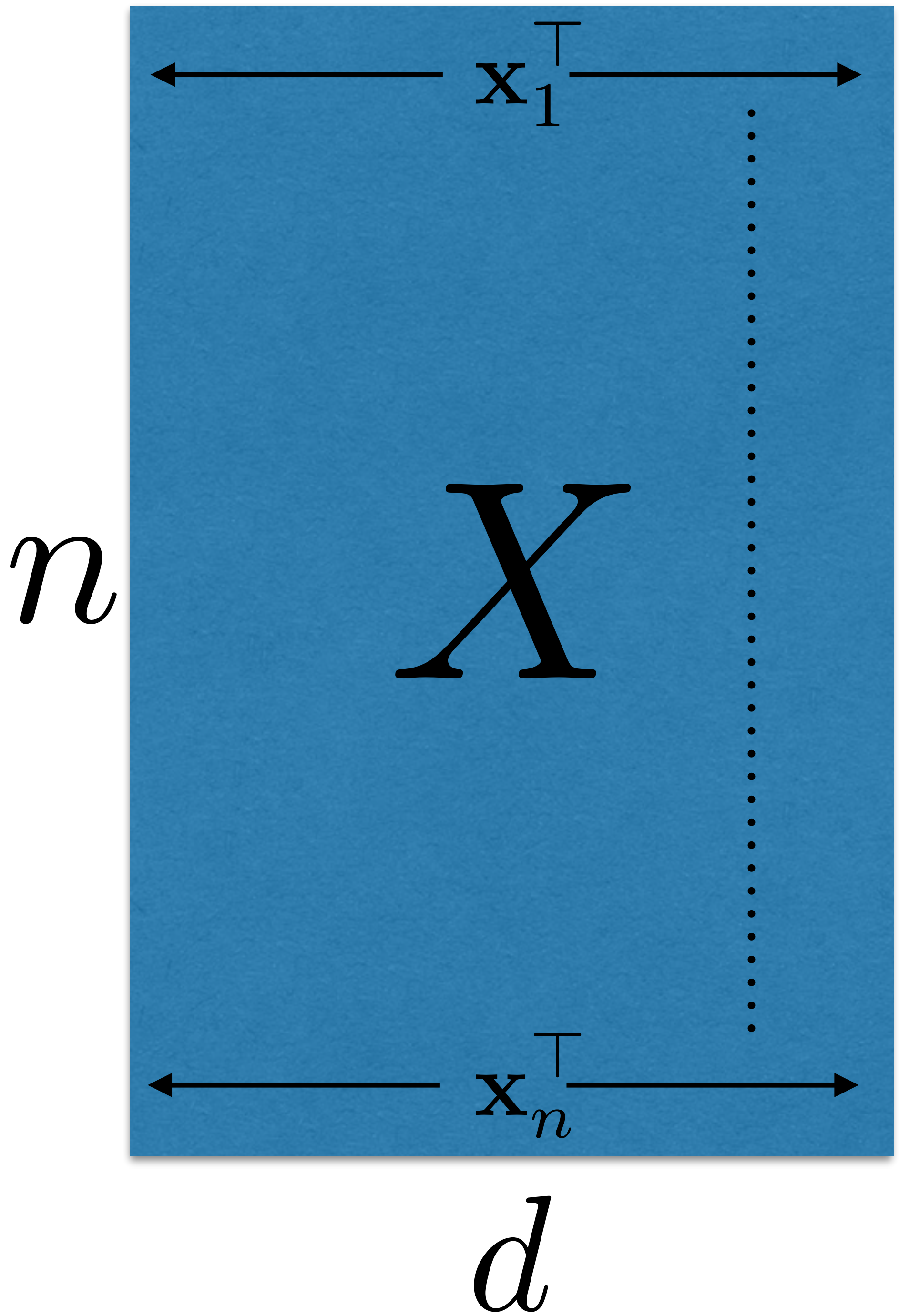
1. Original data can be (approximately) reconstructed
2. Preserve distances between data points
3. "Relevant" information is preserved
4. Noise is reduced

Dim Reduction: Linear Transformation

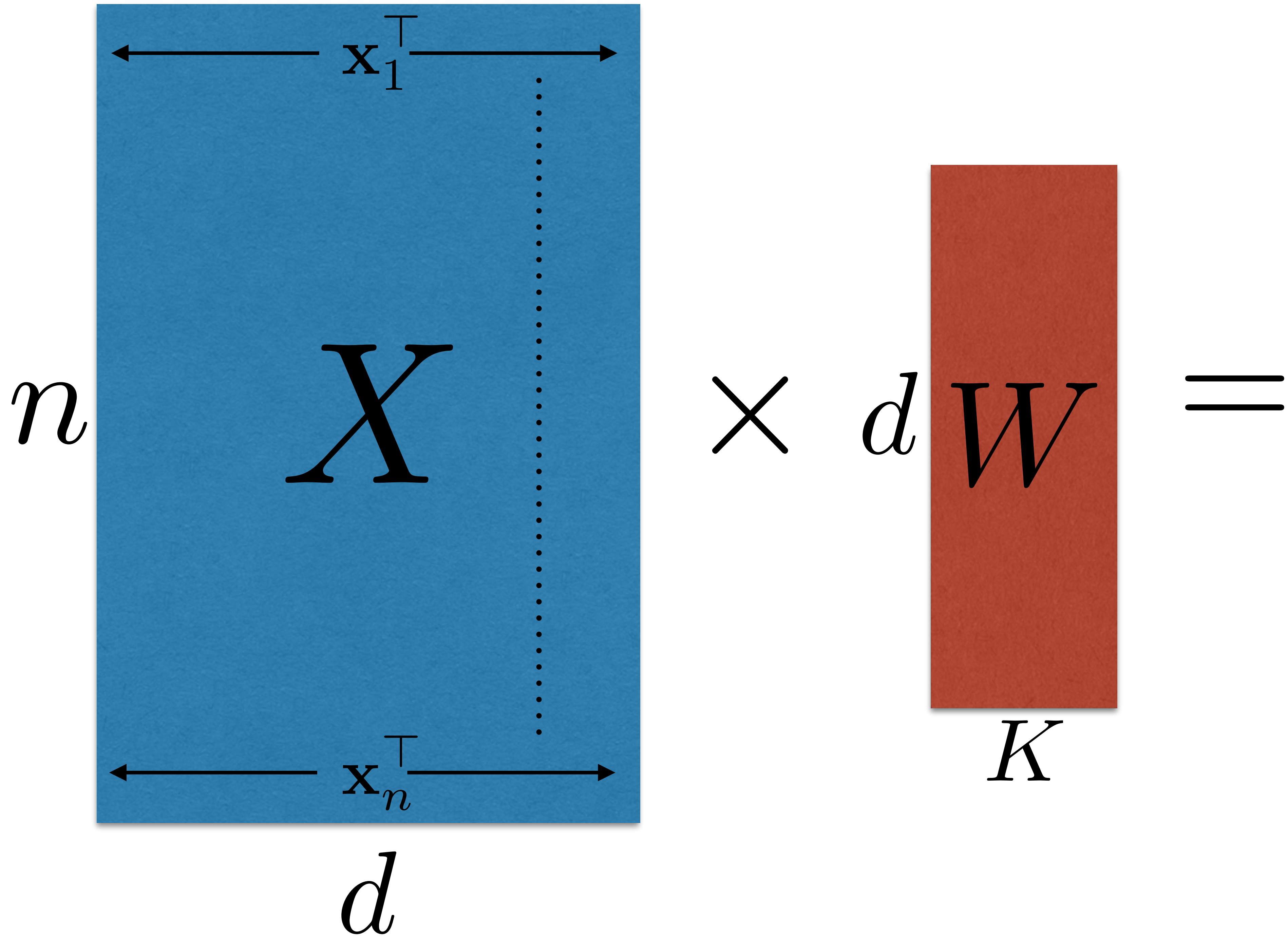
- Pick a low dimensional subspace
- Project linearly to this subspace
- Subspace retains as much information

Dim Reduction: Linear Transformation

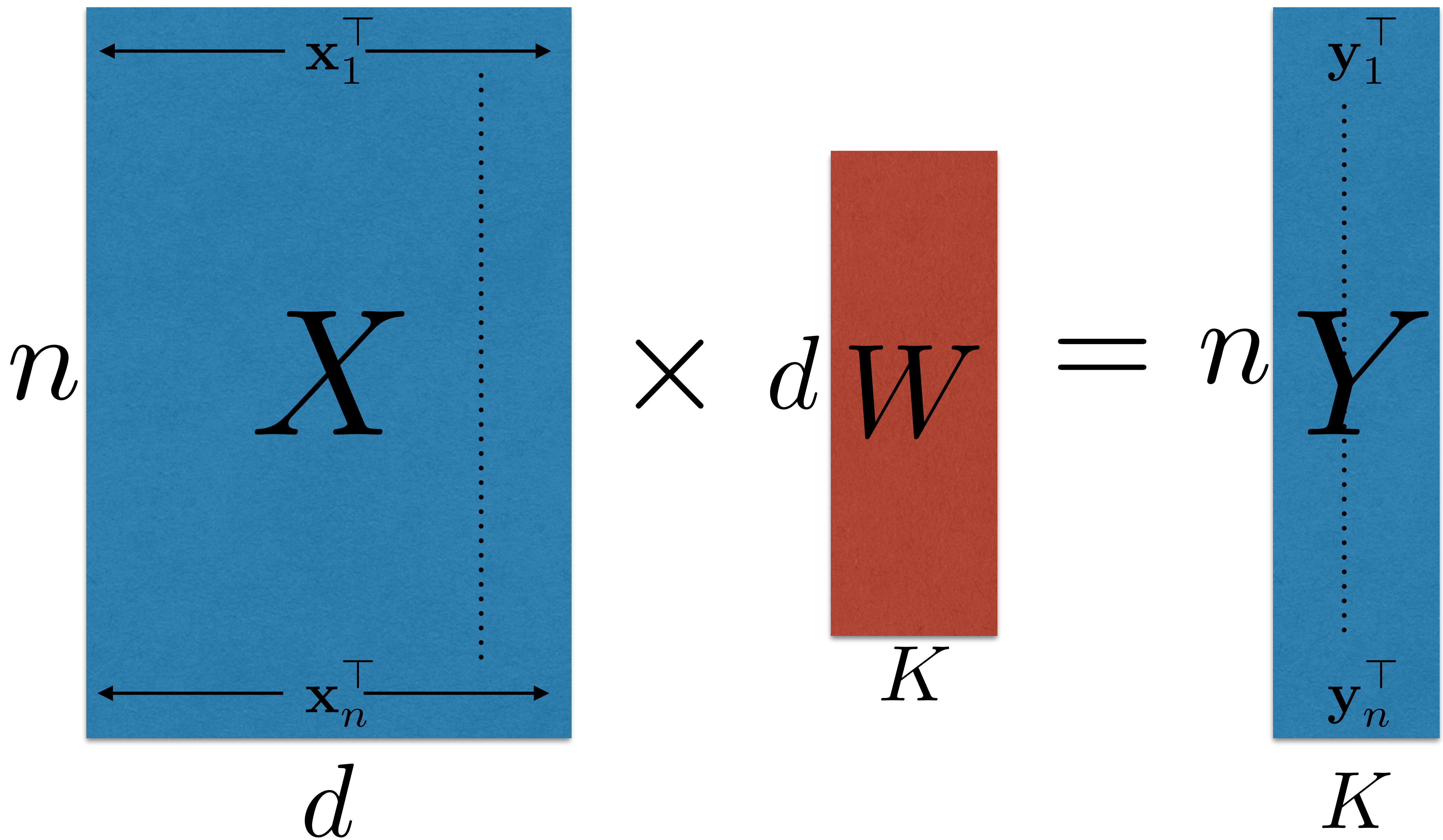
Dim Reduction: Linear Transformation



Dim Reduction: Linear Transformation



Dim Reduction: Linear Transformation



DIM REDUCTION: LINEAR TRANSFORMATION

$$X = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1.1 & 2 & 3 & 4 \\ 3 & 2 & 3 & 4 \\ -1 & 2 & 3 & 4 \\ -0.2 & 2 & 3 & 4 \\ -2 & 2 & 3 & 4 \\ 1.4 & 2 & 3 & 4 \\ 1.4 & 2 & 3 & 4 \\ -0.1 & 2 & 3 & 4 \\ 0.5 & 2 & 3 & 4 \end{bmatrix}$$

Dim Reduction: Linear Transformation

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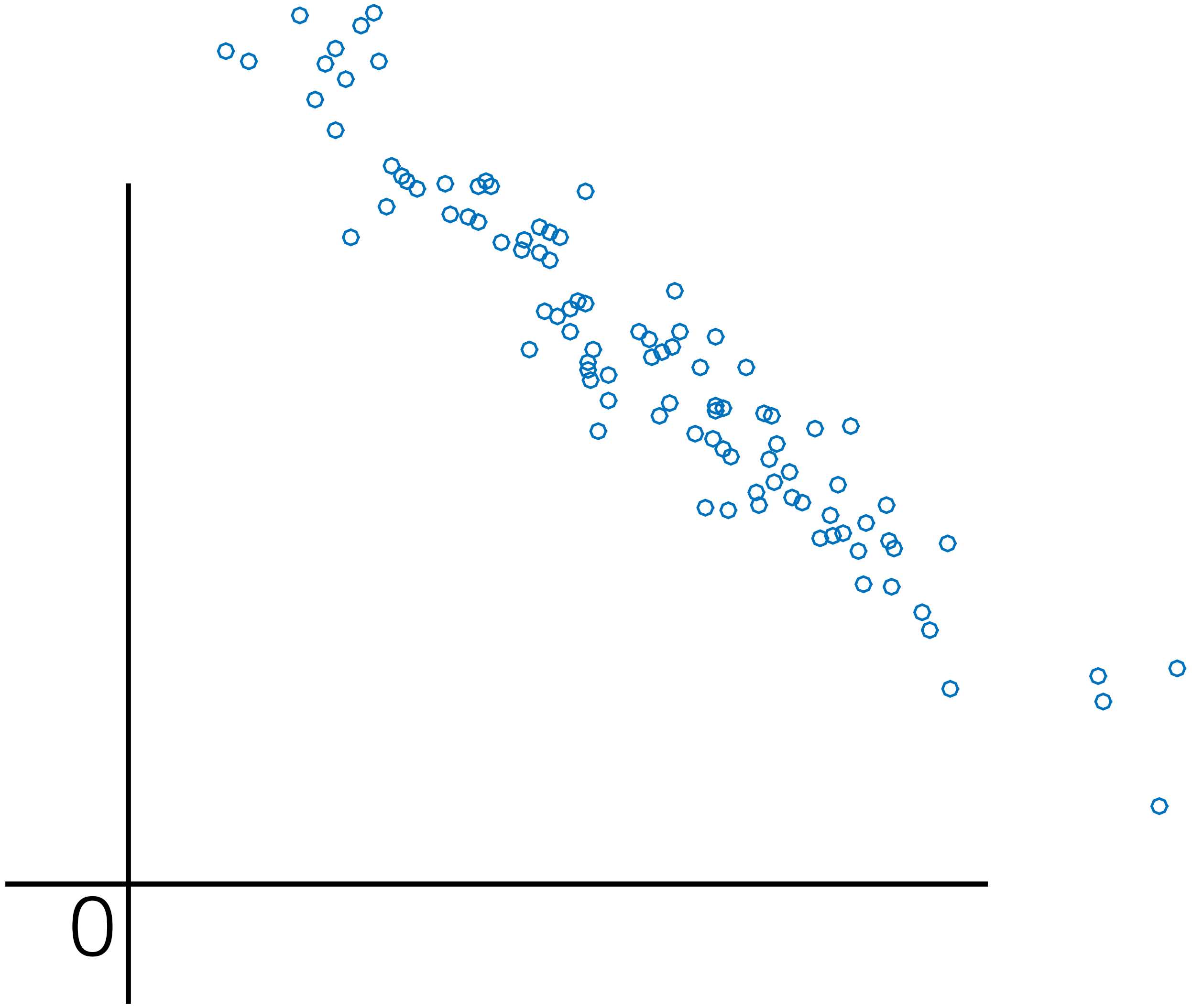
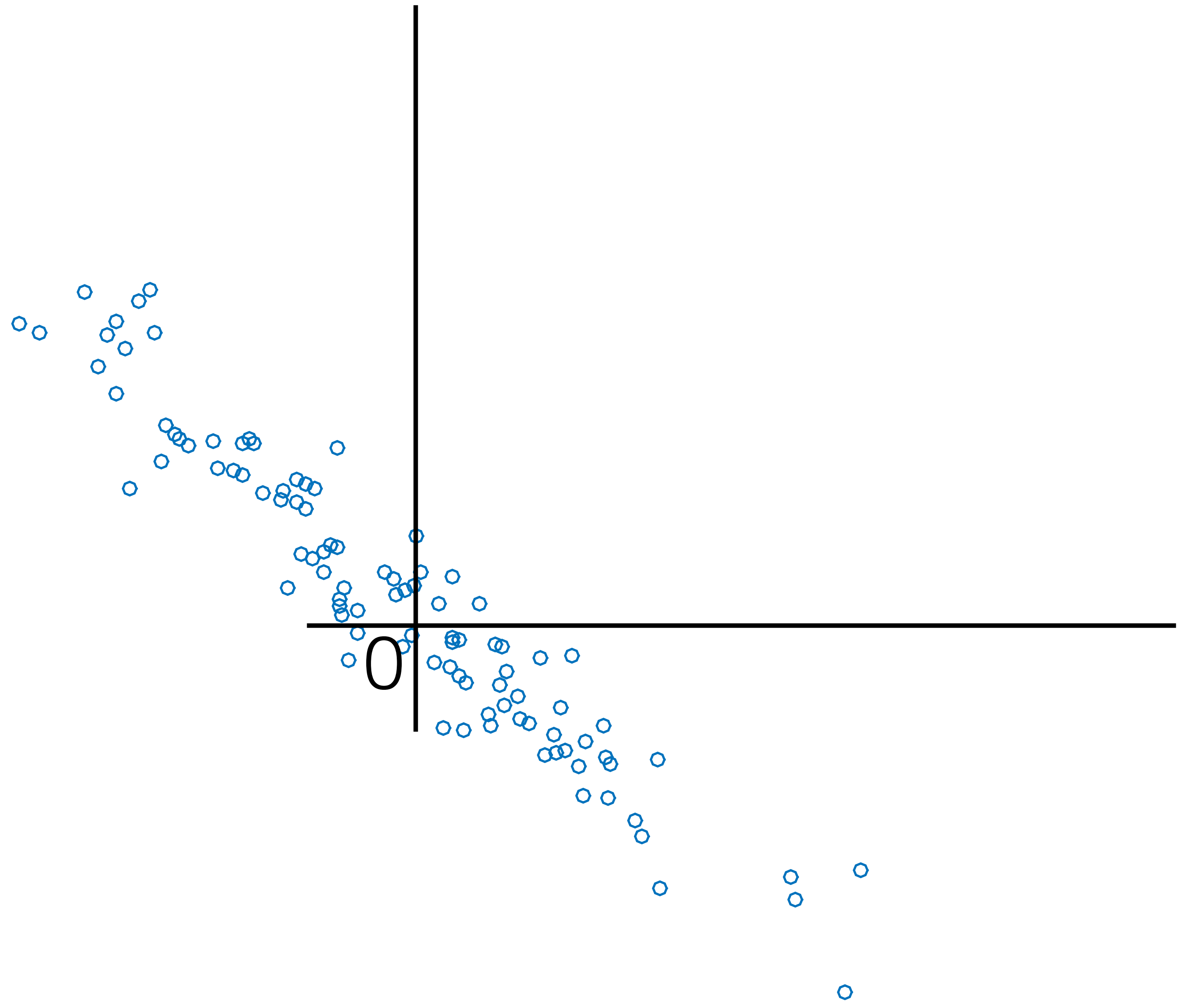
Centering Data



Compressing these data points…

Centering Data

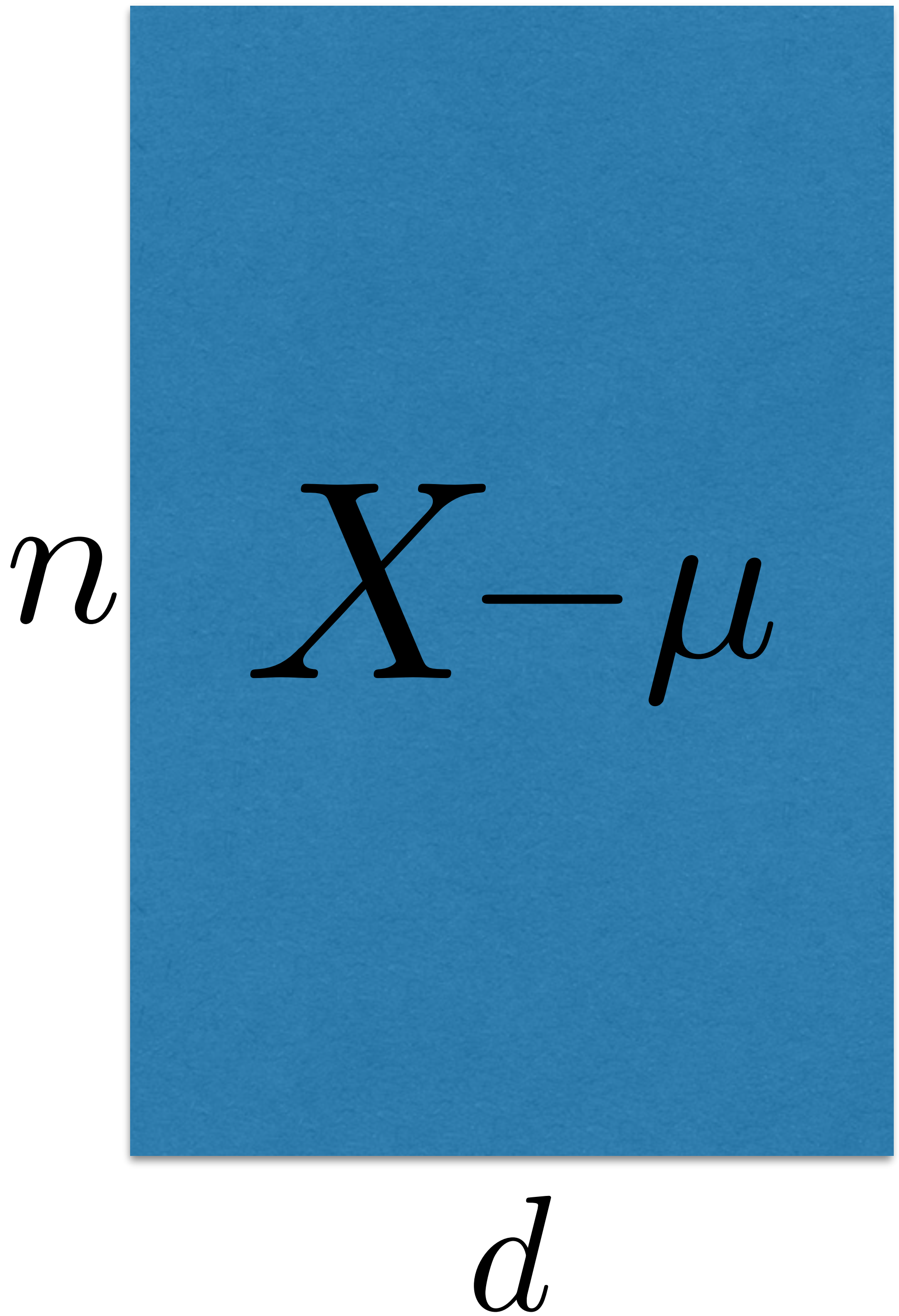


… is same as compressing these.

Centering Data

$$-\mu$$

CENTERING DATA



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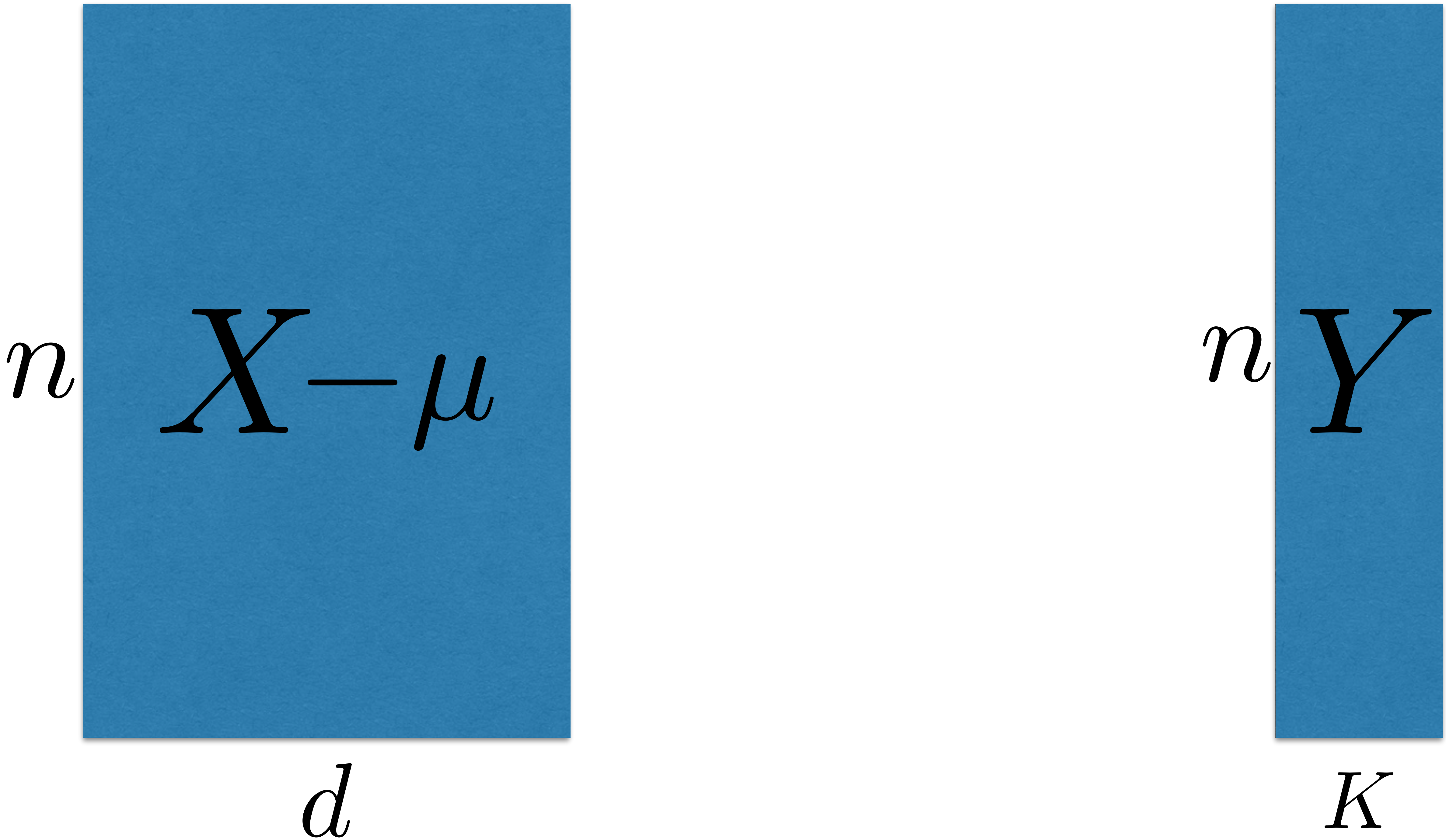

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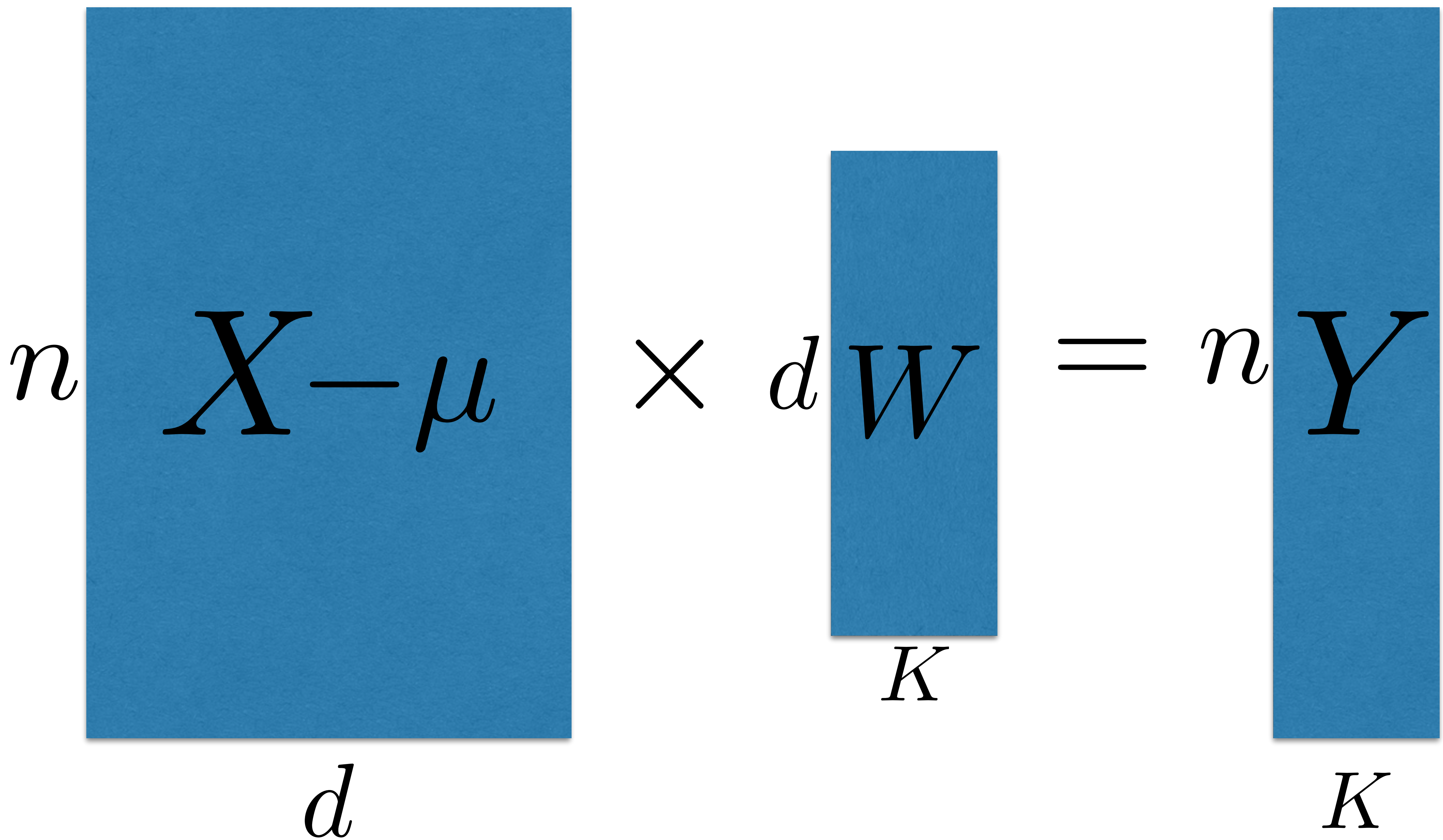
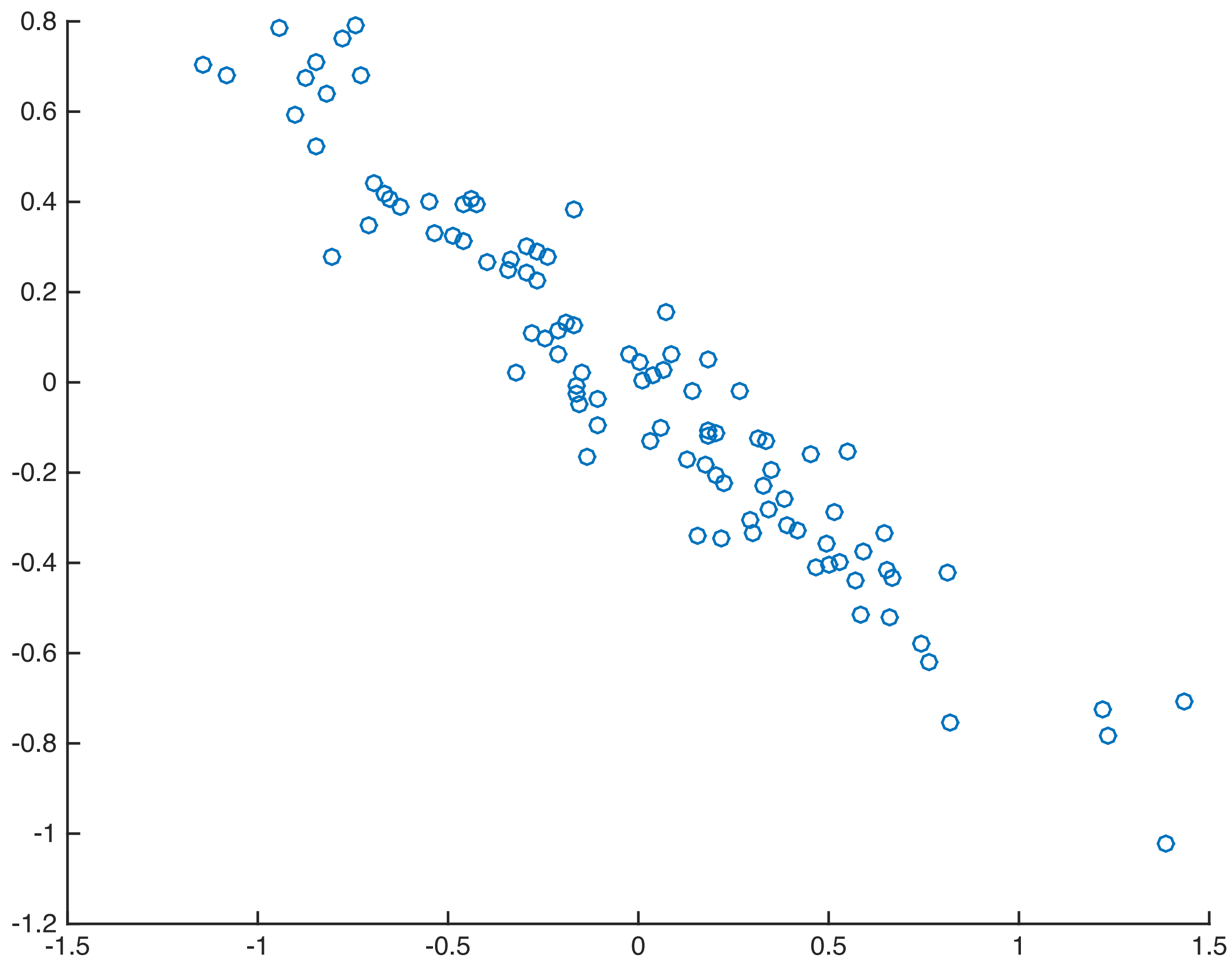


PCA: Variance Maximization



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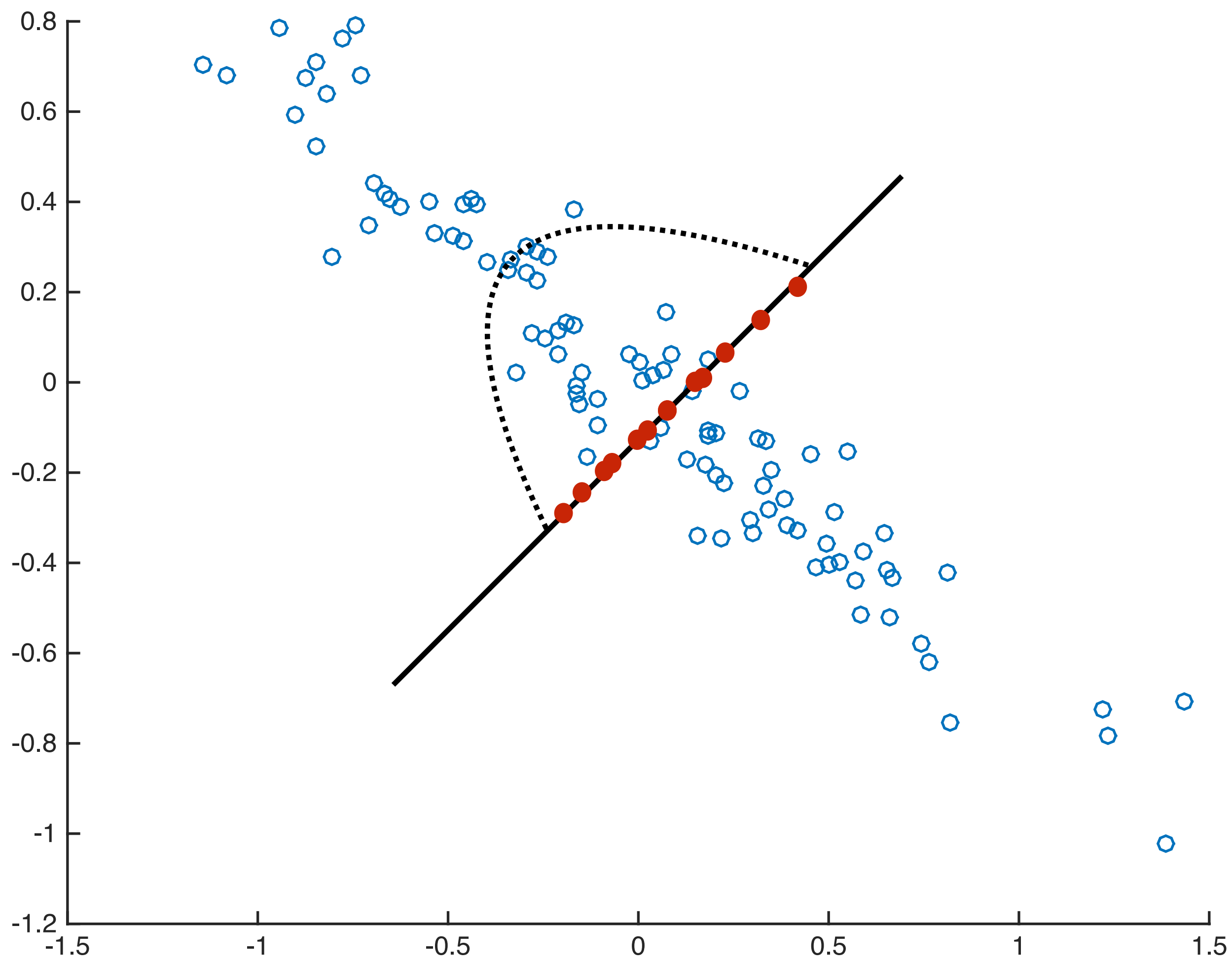

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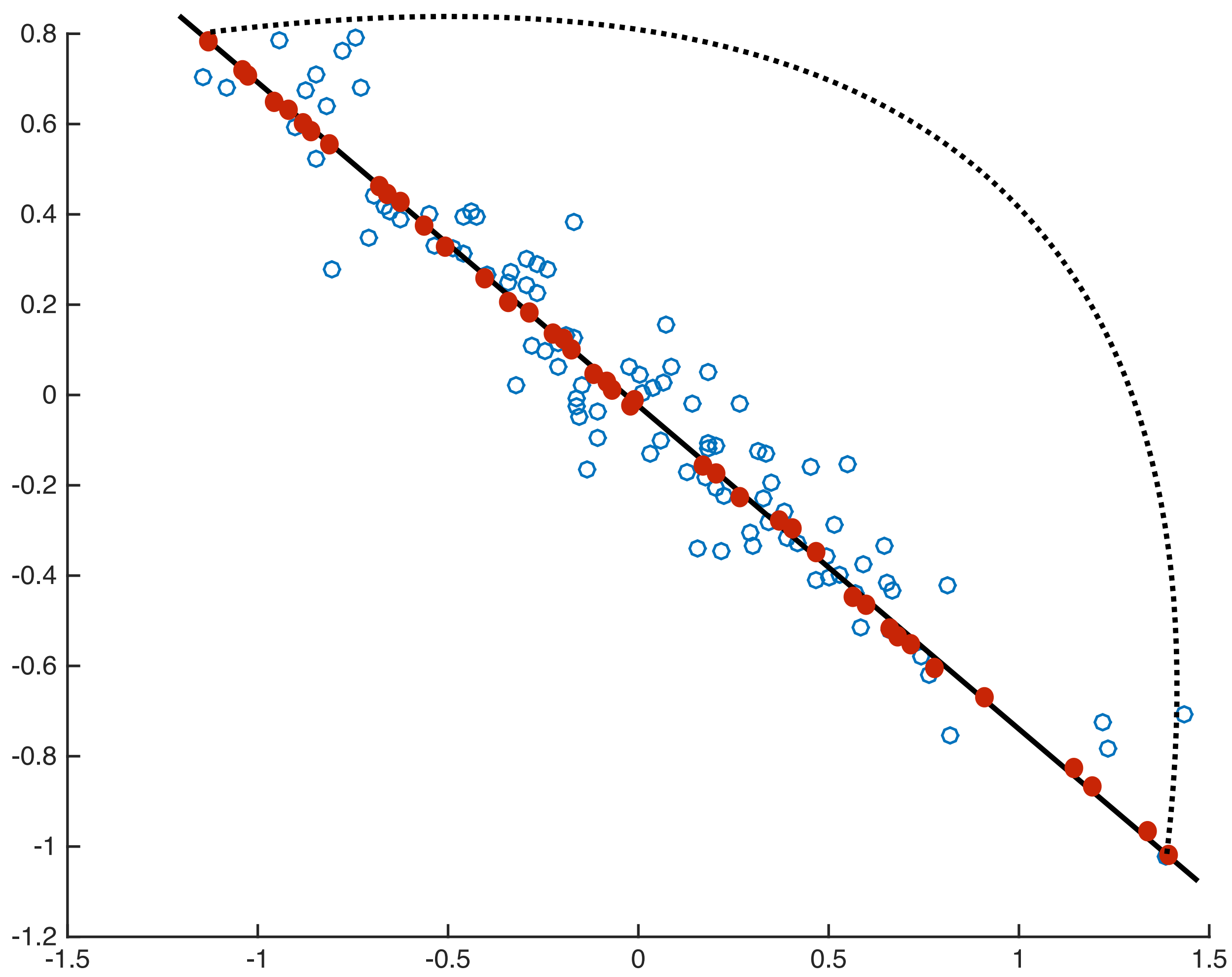

PCA: Variance Maximization

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- First principal component:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}:\|\mathbf{w}\|_2=1} \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top\mathbf{x}_t - \frac{1}{n}\sum_{t=1}^{n}\mathbf{w}^\top\mathbf{x}_t\right)^2$$

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\begin{aligned}
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&= \arg\max_{\mathbf{w}:\|\mathbf{w}\|_2=1} \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top (\mathbf{x}_t - \mu)\right)^2
\end{aligned}
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&= \arg\max_{\mathbf{w}:\|\mathbf{w}\|_2=1} \frac{1}{n}\sum_{t=1}^{n}\mathbf{w}^\top (\mathbf{x}_t - \mu)(\mathbf{x}_t - \mu)^\top \mathbf{w}
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$$= \arg\max_{\mathbf{w}:\|\mathbf{w}\|_2=1} \mathbf{w}^\top\Sigma\mathbf{w}$$

Σ is the covariance matrix

PCA: Variance Maximization

Covariance matrix:

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- Its a $d \times d$ matrix, $\Sigma[i, j]$ measures "covariance" of features i and j

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- Recall $\text{cov}(A, B) = \mathbb{E}[(A - \mathbb{E}[A])(B - \mathbb{E}[B])]$

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- Recall $\mathrm{cov}(A,B) = \mathbb{E}[(A - \mathbb{E}[A])(B - \mathbb{E}[B])]$
- Alternatively,

$$\Sigma[i,j] = \frac{1}{n}\begin{bmatrix} \mathbf{x}_1[j] - \mu[j] \\ \mathbf{x}_2[j] - \mu[j] \\ \cdots \\ \cdots \\ \cdots \\ \mathbf{x}_n[j] - \mu[j] \end{bmatrix}^\top \begin{bmatrix} \mathbf{x}_1[j] - \mu[j] \\ \mathbf{x}_2[j] - \mu[j] \\ \cdots \\ \cdots \\ \cdots \\ \mathbf{x}_n[j] - \mu[j] \end{bmatrix}$$

Inner products measure similarity.

PCA: Variance Maximization

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To solve the above maximization problem, we use Lagrange multipliers. Specifically there exists λ such that solution $\mathbf{w}_1$ is:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \Sigma \mathbf{w} - \lambda \|\mathbf{w}\|_2^2$$

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Taking derivate and equality to 0 we find that $\Sigma \mathbf{w} = \lambda \mathbf{w}$ (ie. eigenvector). Plugging this back into Eq. 1,

$$\frac{1}{n} \sum_{t=1}^{n} \mathbf{w}^\top \Sigma \mathbf{w} = \mathbf{w}^\top (\lambda \mathbf{w}) = \lambda$$

Hence to maximize variance we pick direction with largest eigenvalue

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- Eigenvectors of the covariance matrix are the principal components

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PRINCIPAL COMPONENT ANALYSIS

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Principal Component Analysis

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- Top K principal components are the eigenvectors with K largest eigenvalues
- Projection = Data × Top K eigenvectors
- Reconstruction = Projection × Transpose of top K eigenvectors
- Independently discovered by Pearson in 1901 and Hotelling in 1933.

Principal Component Analysis: Demo