Machine Learning for Data Science (CS4786)
Lecture 2

Dimensionality Reduction
&
Principal Component Analysis

Quiz

- Let Σ be the empirical covariance matrix of n points in d dimensions

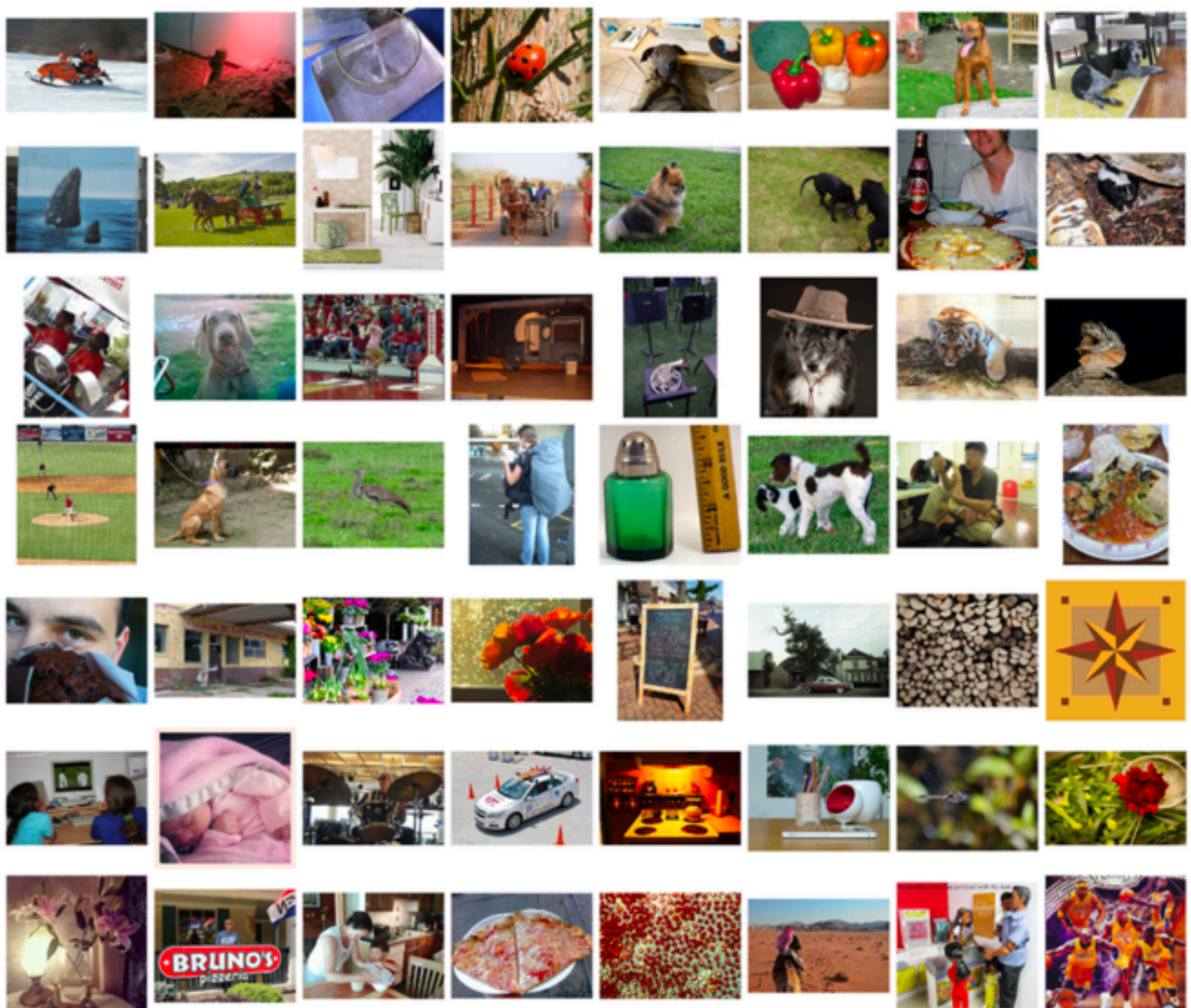
A. Σ is an n x n matrix

B. Σ is a d x d matrix

C. Σ is a m x m matrix where m is the underlying dimensionality of the n points (which can be at most d)

D. rank(Σ) is m where m is the underlying dimensionality of the n points

We can compress the following images using JPEG?

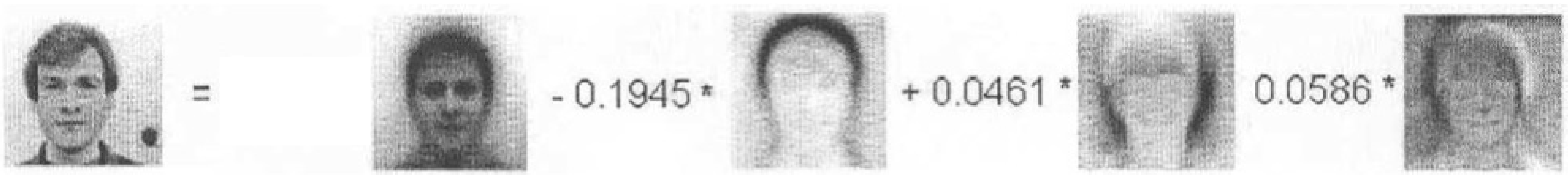


What if our dataset looked like this?

Principal Component Analysis (PCA)

Turk & Pentland'91

Eigen Face:



PRINCIPAL COMPONENT ANALYSIS (PCA)

Turk & Pentland'91

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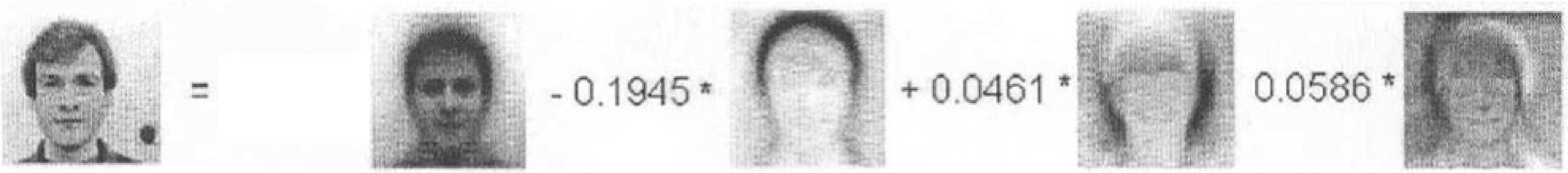

- Write down each data point as a linear combination of small number of basis vectors

PRINCIPAL COMPONENT ANALYSIS (PCA)

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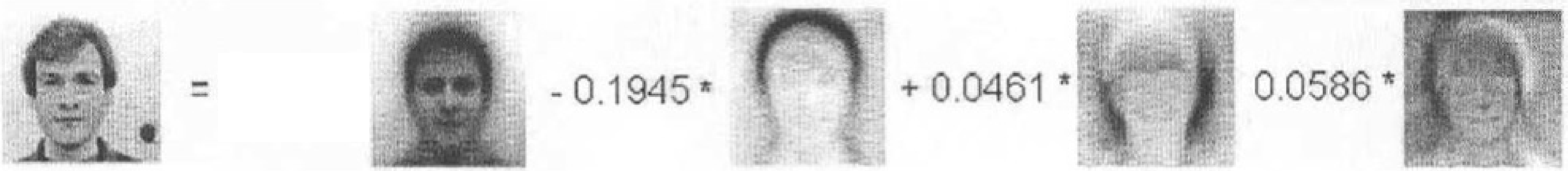

- Write down each data point as a linear combination of small number of basis vectors

- Data specific compression scheme

PRINCIPAL COMPONENT ANALYSIS (PCA)

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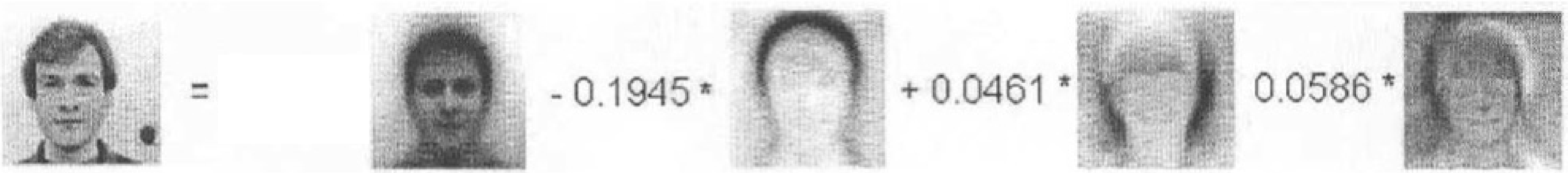


- Write down each data point as a linear combination of small number of basis vectors
- Data specific compression scheme
- One of the early successes: in face recognition: classification based on nearest neighbor in the reduced dimension space

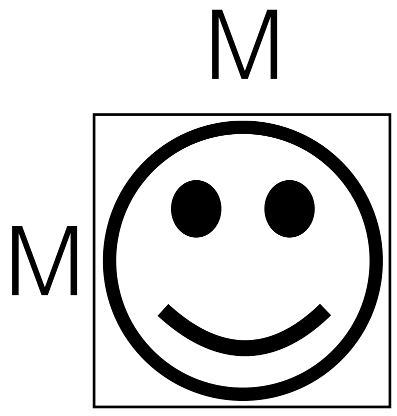
Representing Data as Feature Vectors

- How do we represent data?

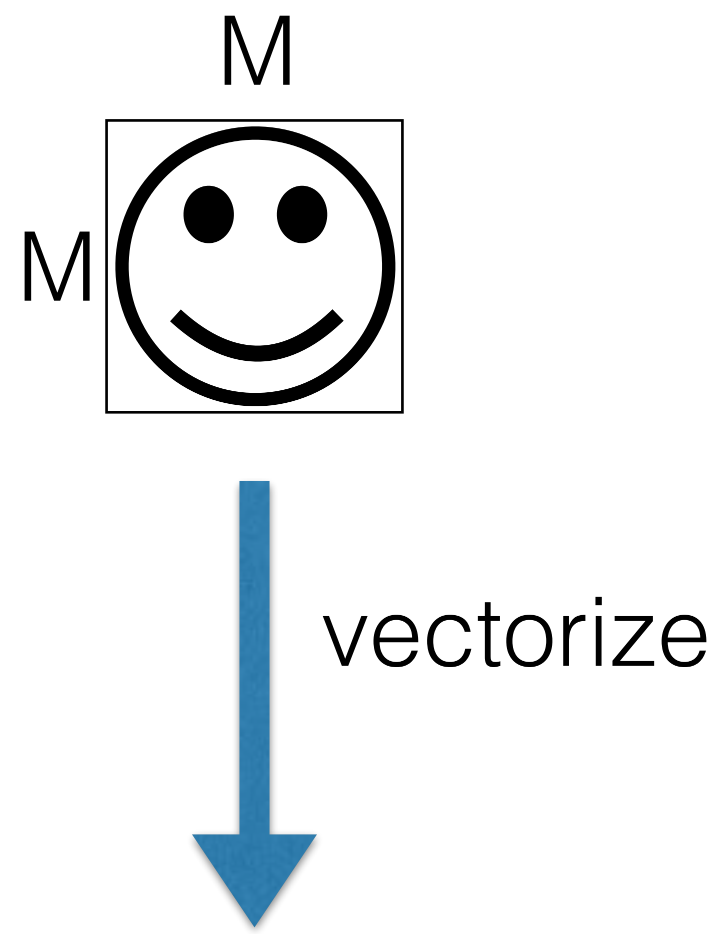
Representing Data as Feature Vectors

- How do we represent data?
- Each data-point often represented as vector referred to as feature vector

Example: Images



Example: Images



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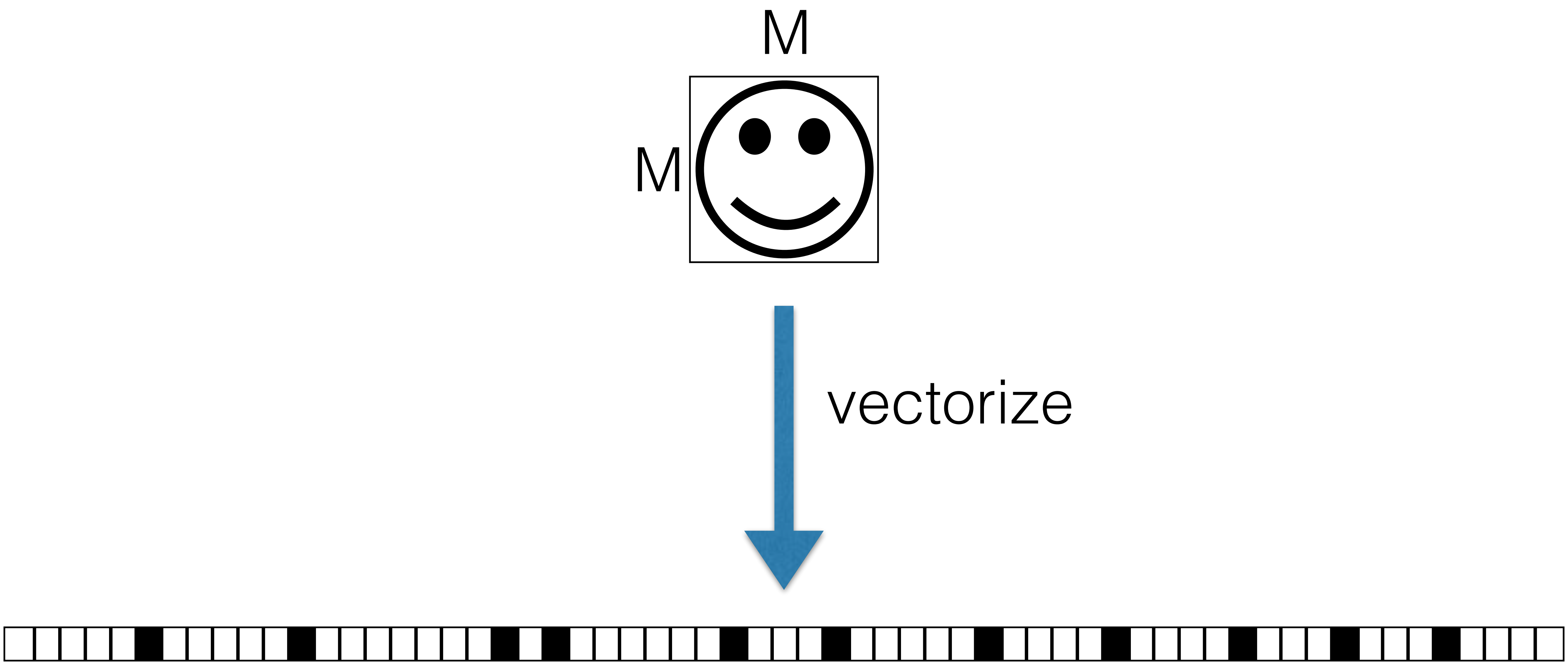

$d = M^2$

Example: Text (Bag of Words)

Documents:

car
engine
hood
tires
truck
trunk

car
emissions
hood
make
model
trunk

Chomsky
corpus
noun
parsing
tagging
wonderful

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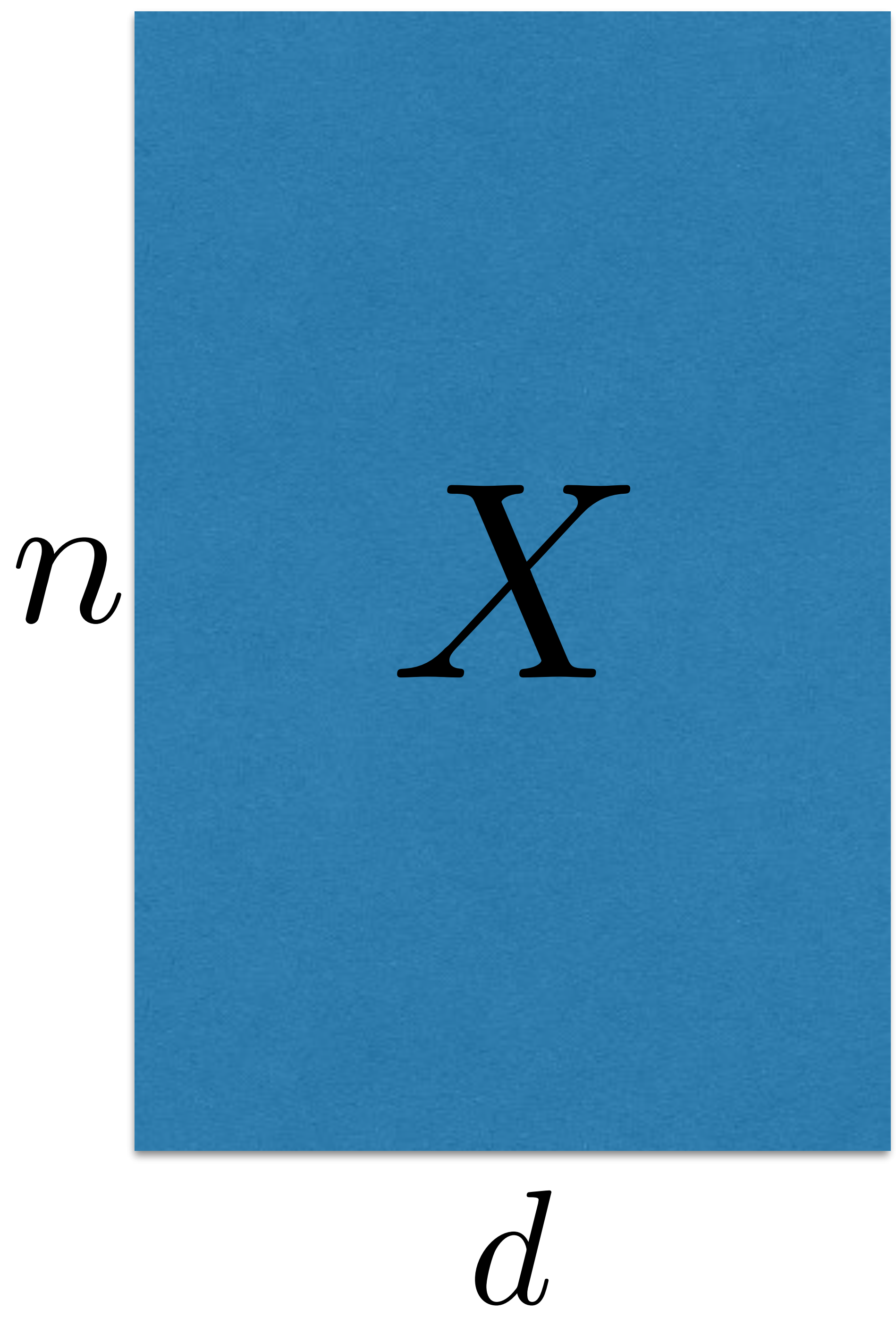
car	Chomsky	corpus	emissions	engine	hood	make	model	noun	parsing	tagging	tires	truck	trunk	wonderful
1	0	0	0	1	1	0	0	0	0	0	1	1	1	0
1	0	0	1	0	1	1	1	0	0	0	0	0	1	0
0	1	1	0	0	0	0	0	1	1	1	0	0	0	1

Dimensionality Reduction

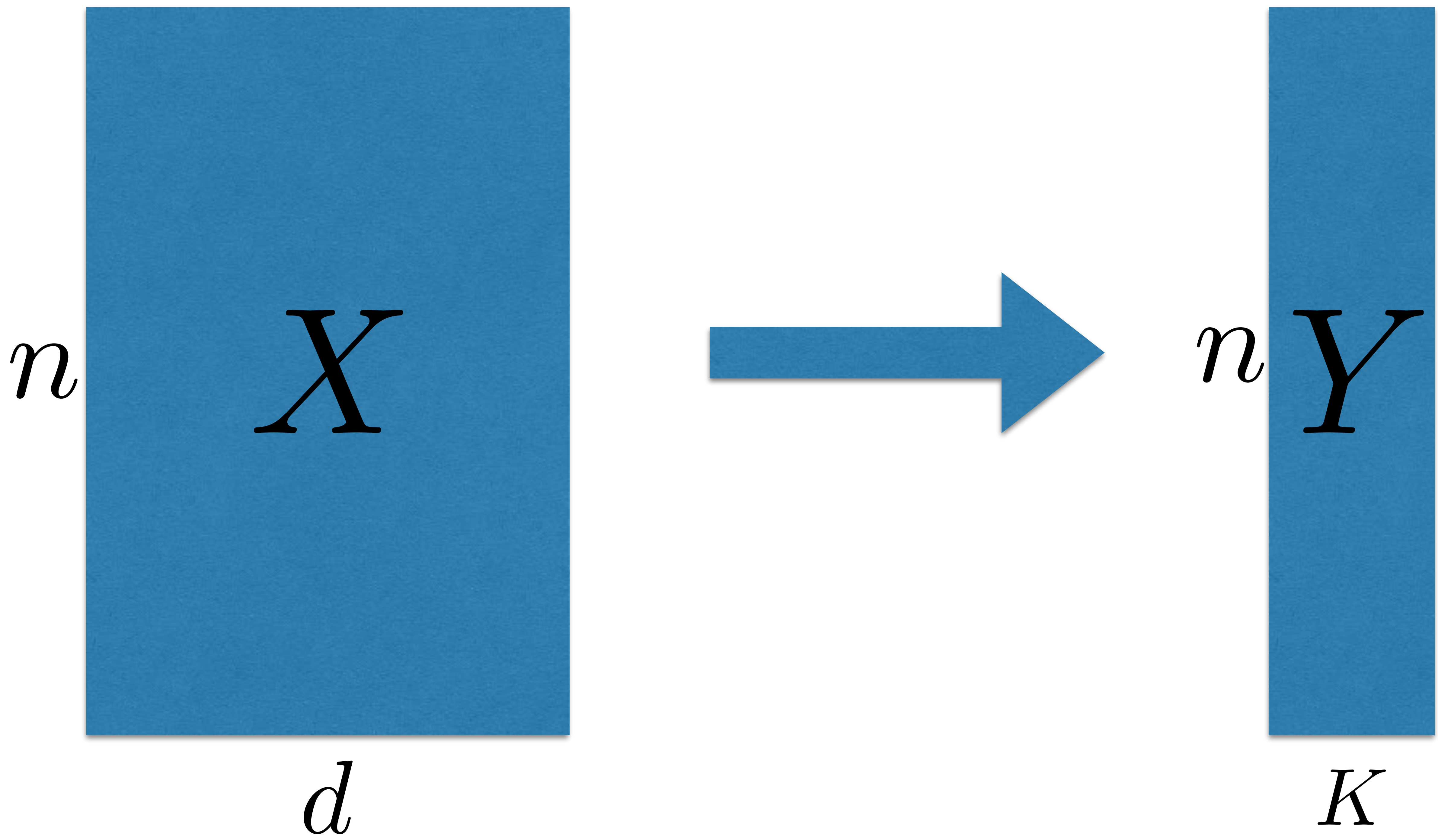
Given n data points in high-dimensional space, compress them into corresponding n points in lower dimensional space.

Dimensionality Reduction

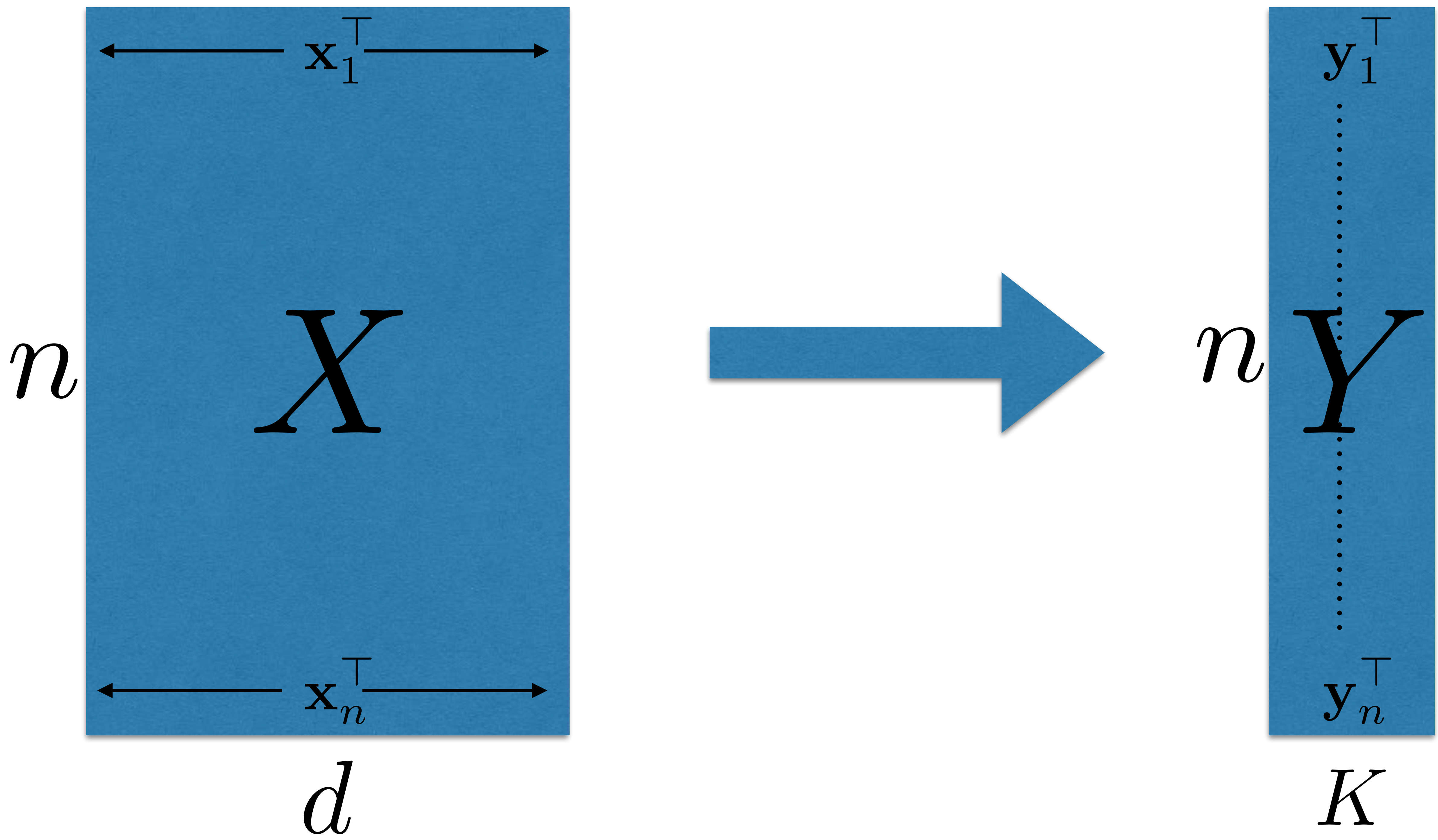
Dimensionality Reduction



Dimensionality Reduction



Dimensionality Reduction



Why dimensionality reduction?

- For computational ease
  - As input to supervised learning algorithm
  - Before clustering to remove redundant information and noise
- Data compression & Noise reduction
- Data visualization

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

Can we reduce to 1 dim?

0.95225911	-1.90451821	2.85677732
0.60681578	-1.21363156	1.82044733
0.76419773	-1.52839546	2.29259318
0.44430217	-0.88860435	1.33290652
0.98425485	-1.9685097	2.95276456
0.04590113	-0.09180227	0.1377034
0.52408131	-1.04816263	1.57224394
0.2887897	-0.5775794	0.8663691
0.4289135	-0.857827	1.2867405
0.23877452	-0.47754905	0.71632357
0.50031855	-1.00063711	1.50095566
0.7155322	-1.43106441	2.14659661
0.19638816	-0.39277632	0.58916448
0.06743744	-0.13487488	0.20231232
0.18019499	-0.36038997	0.54058496
0.68941225	-1.37882451	2.06823676
0.51882043	-1.03764087	1.5564613
0.71398952	-1.42797904	2.14196857
[illegible]	[illegible]	[illegible]

Example:
Students in classroom

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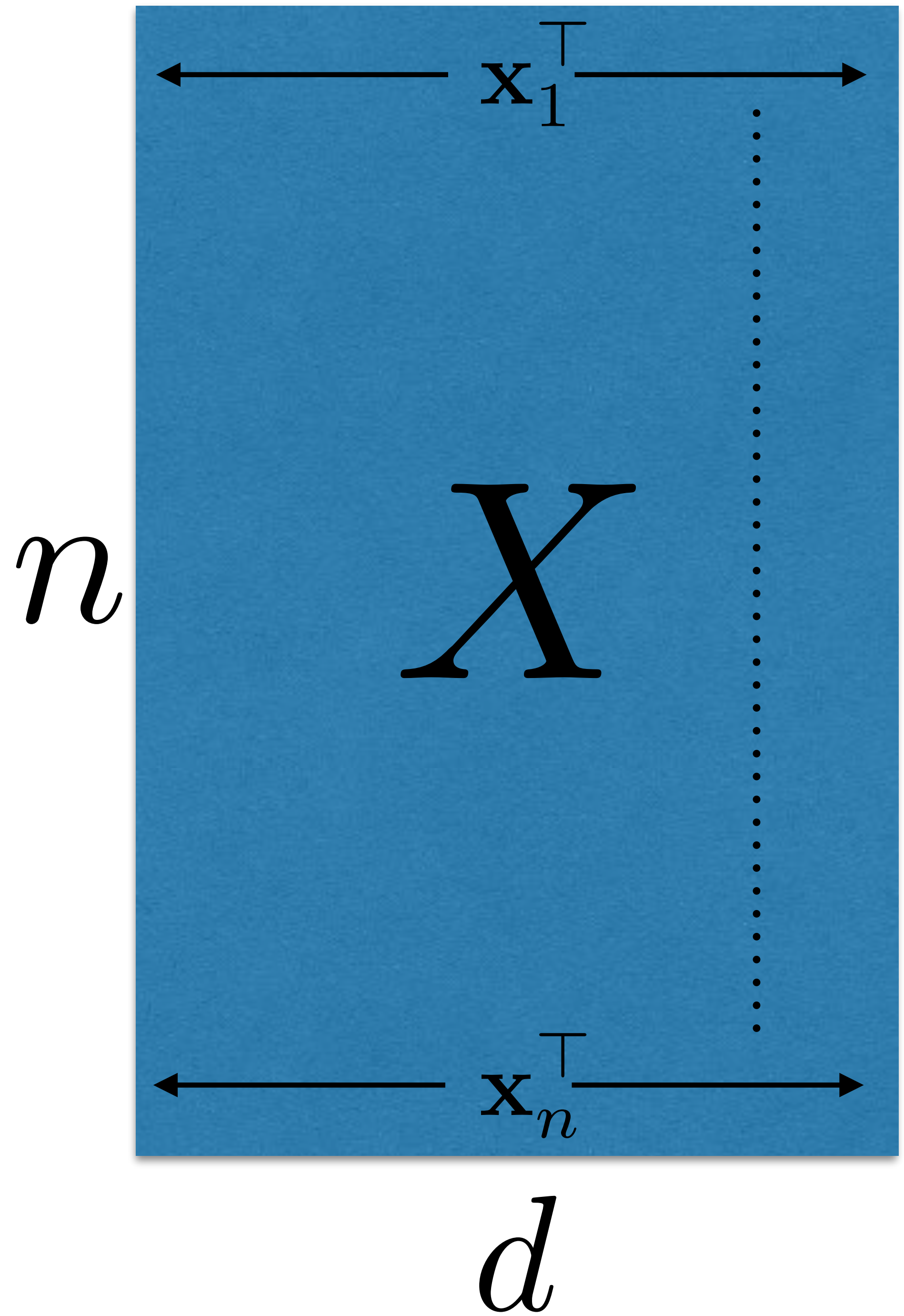
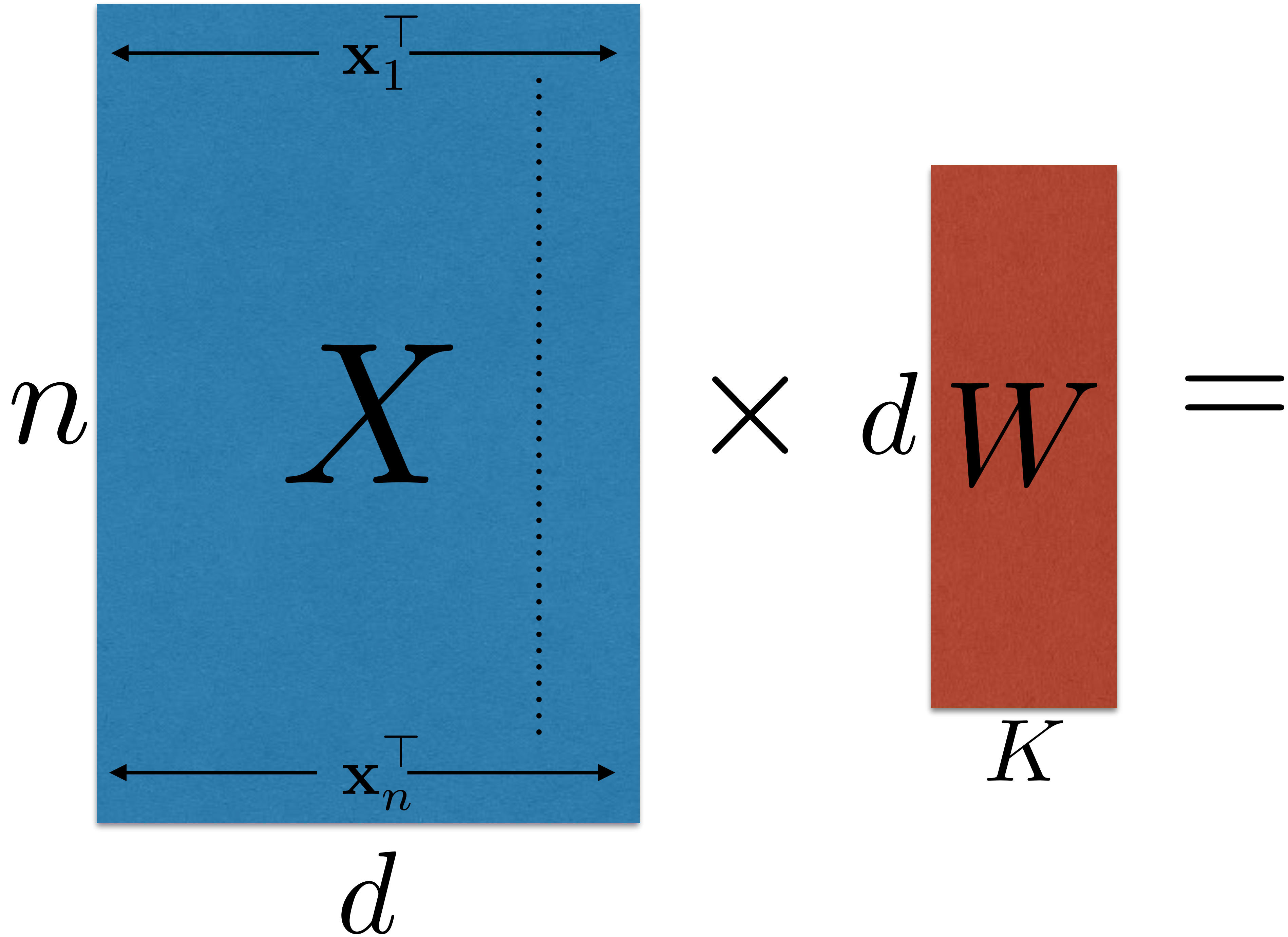
Dim Reduction: Linear Transformation

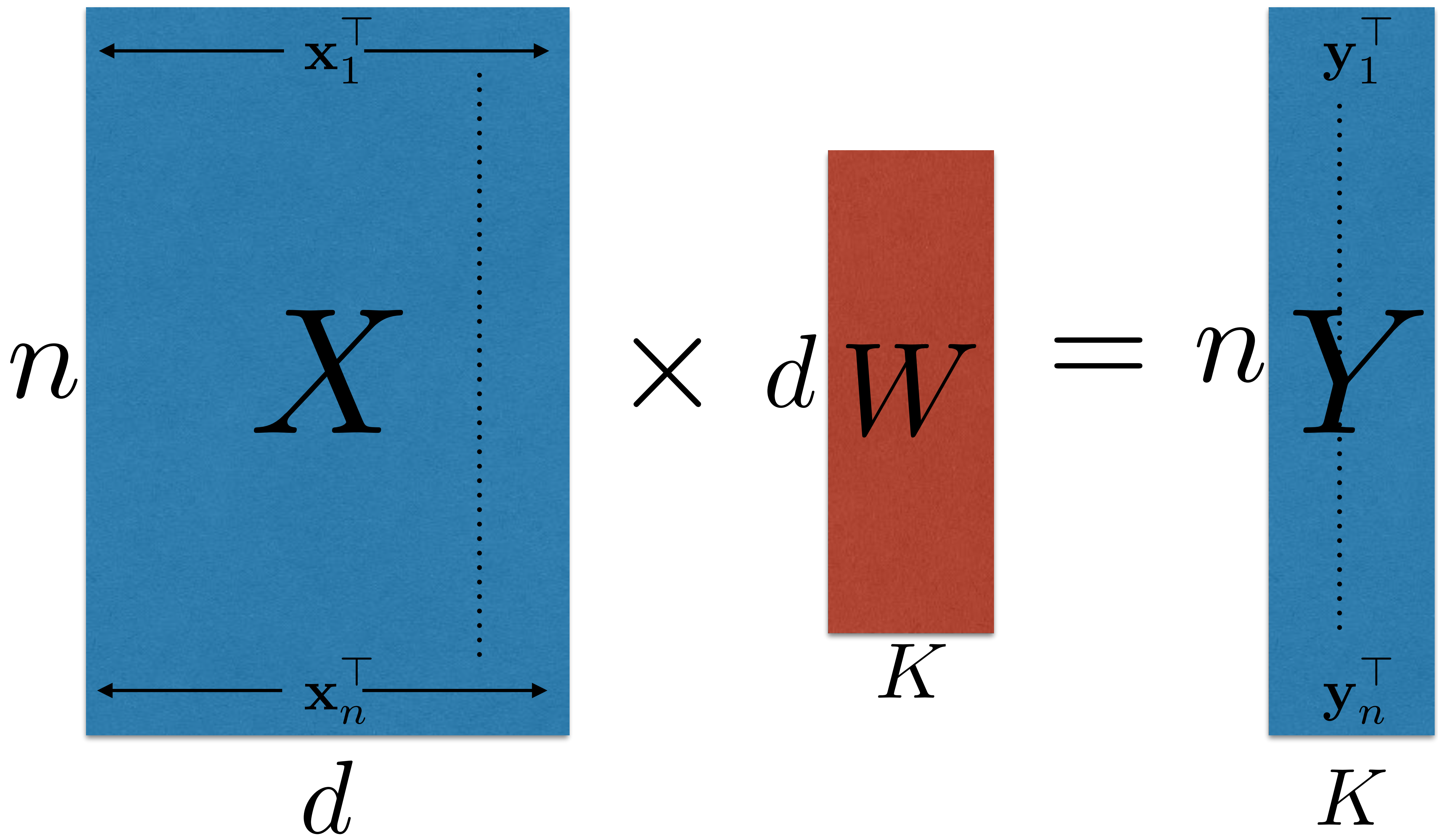
Dim Reduction: Linear Transformation



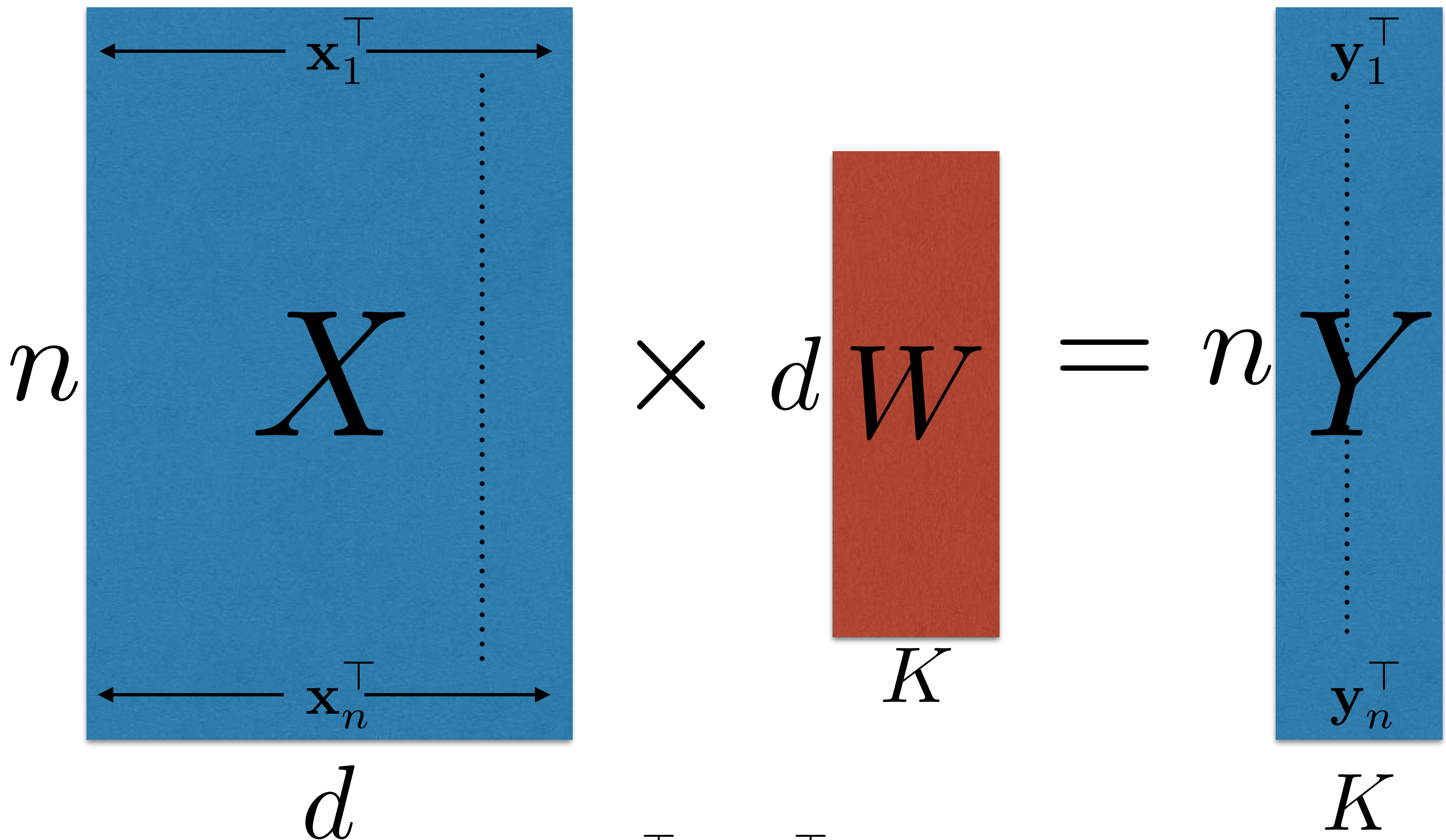
Dim Reduction: Linear Transformation



DIM REDUCTION: LINEAR TRANSFORMATION



Dim Reduction: Linear Transformation

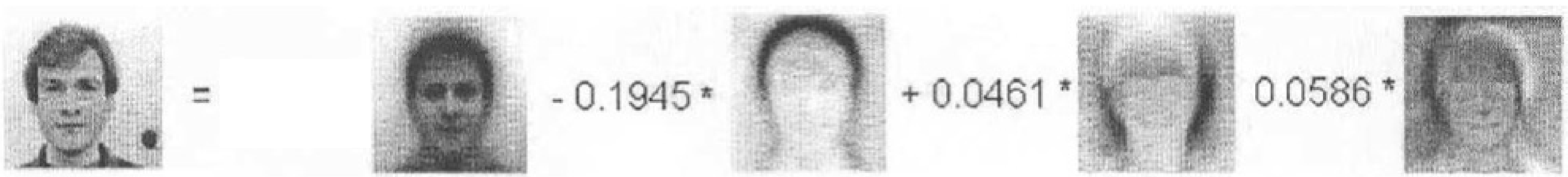


$$\mathbf{y}_i^\top = \mathbf{x}_i^\top W$$

Principal Component Analysis (PCA)

Turk & Pentland'91

Eigen Face:



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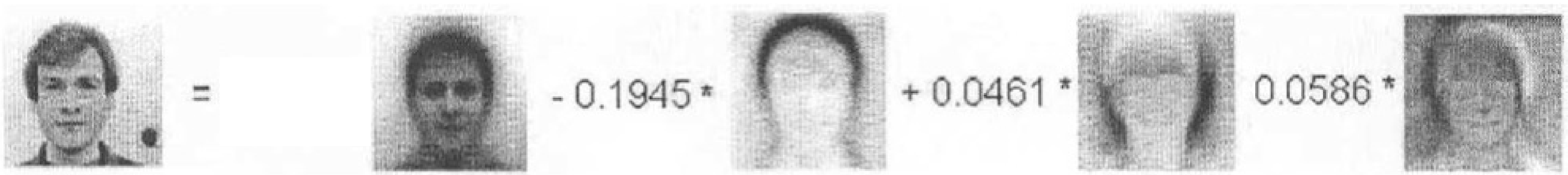

- Each x_t (each row of X) is a face image (vectorized version)

Principal Component Analysis (PCA)

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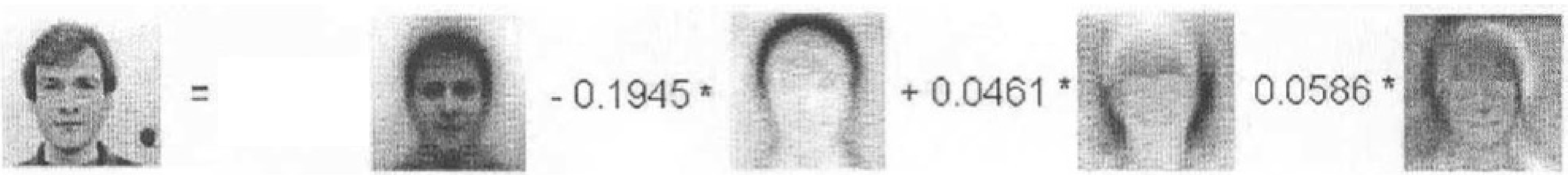

- Each x_t (each row of X) is a face image (vectorized version)
- Each y_t is the set of coefficients we multiply to the eigen face

PRINCIPAL COMPONENT ANALYSIS (PCA)

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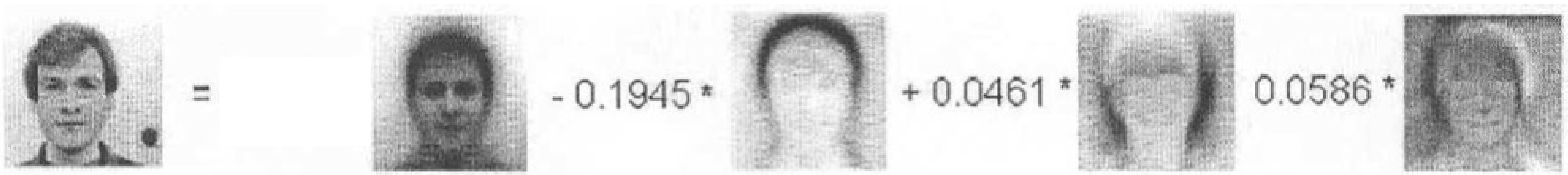
Eigen Face:



- Each x_t (each row of X) is a face image (vectorized version)
- Each y_t is the set of coefficients we multiply to the eigen face
- Each column of W is an Eigenface

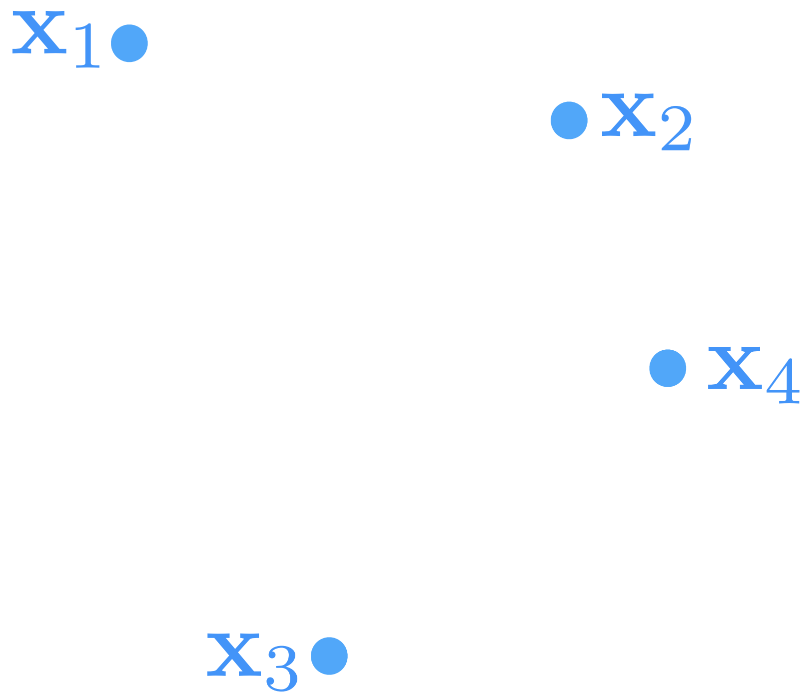
Prelude: Reducing to 1 Dim

- W is a d x 1 matrix (d dimensional vector)
- Each data point is compressed to a single number
- How do we pick this W?

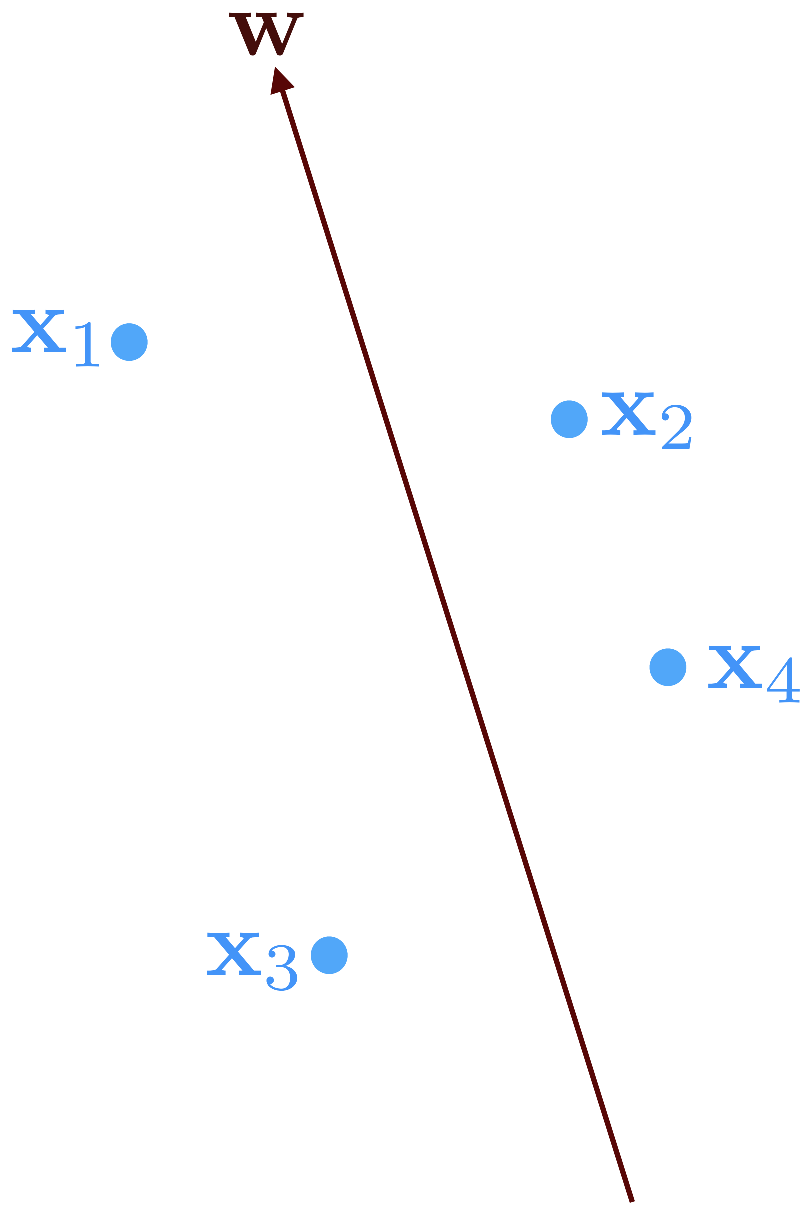
Prelude: reducing to 1 dimension

Dim Reduction: Linear Transformation

Prelude: reducing to 1 dimension



Prelude: reducing to 1 dimension



Dim Reduction: Linear Transformation

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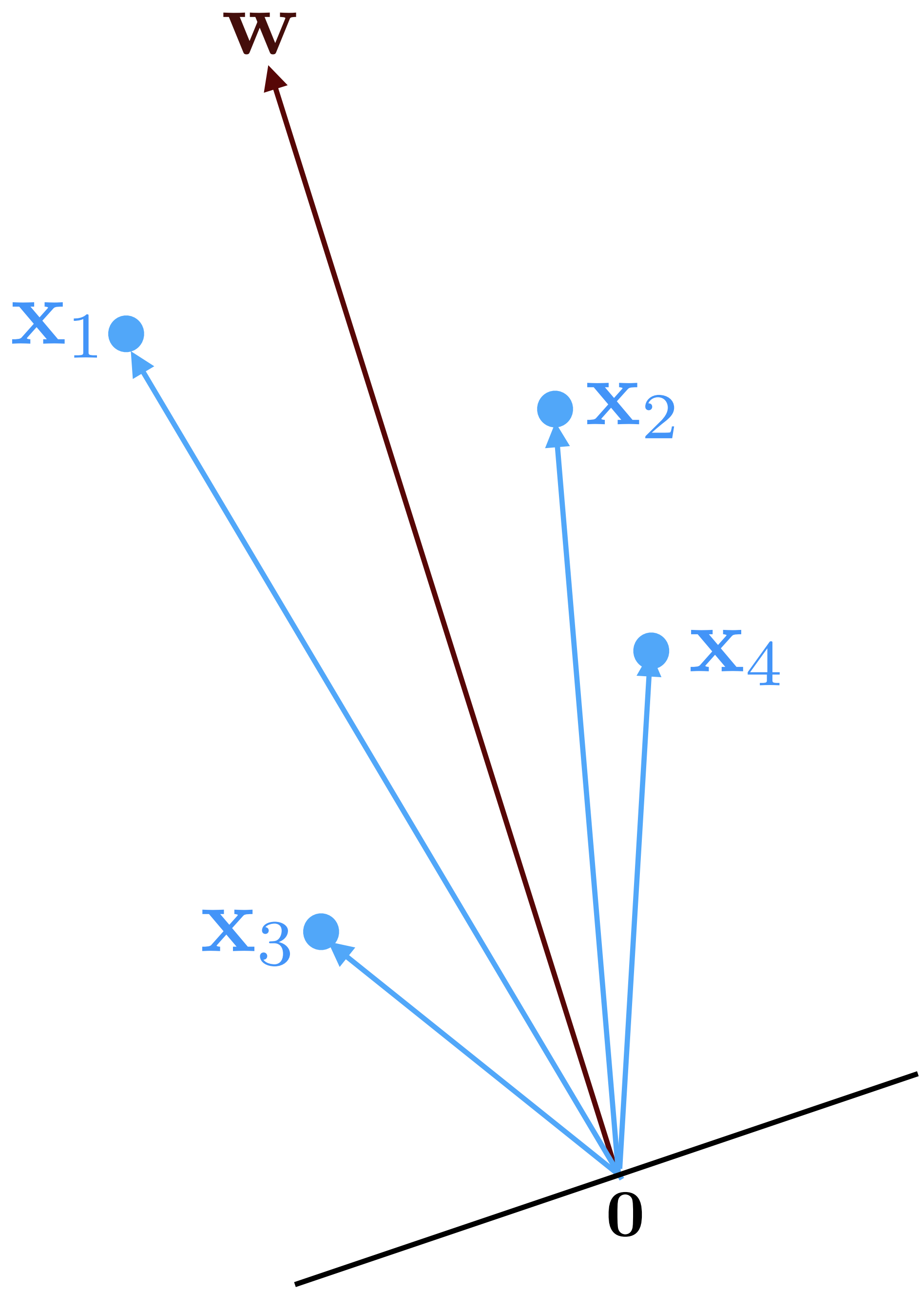
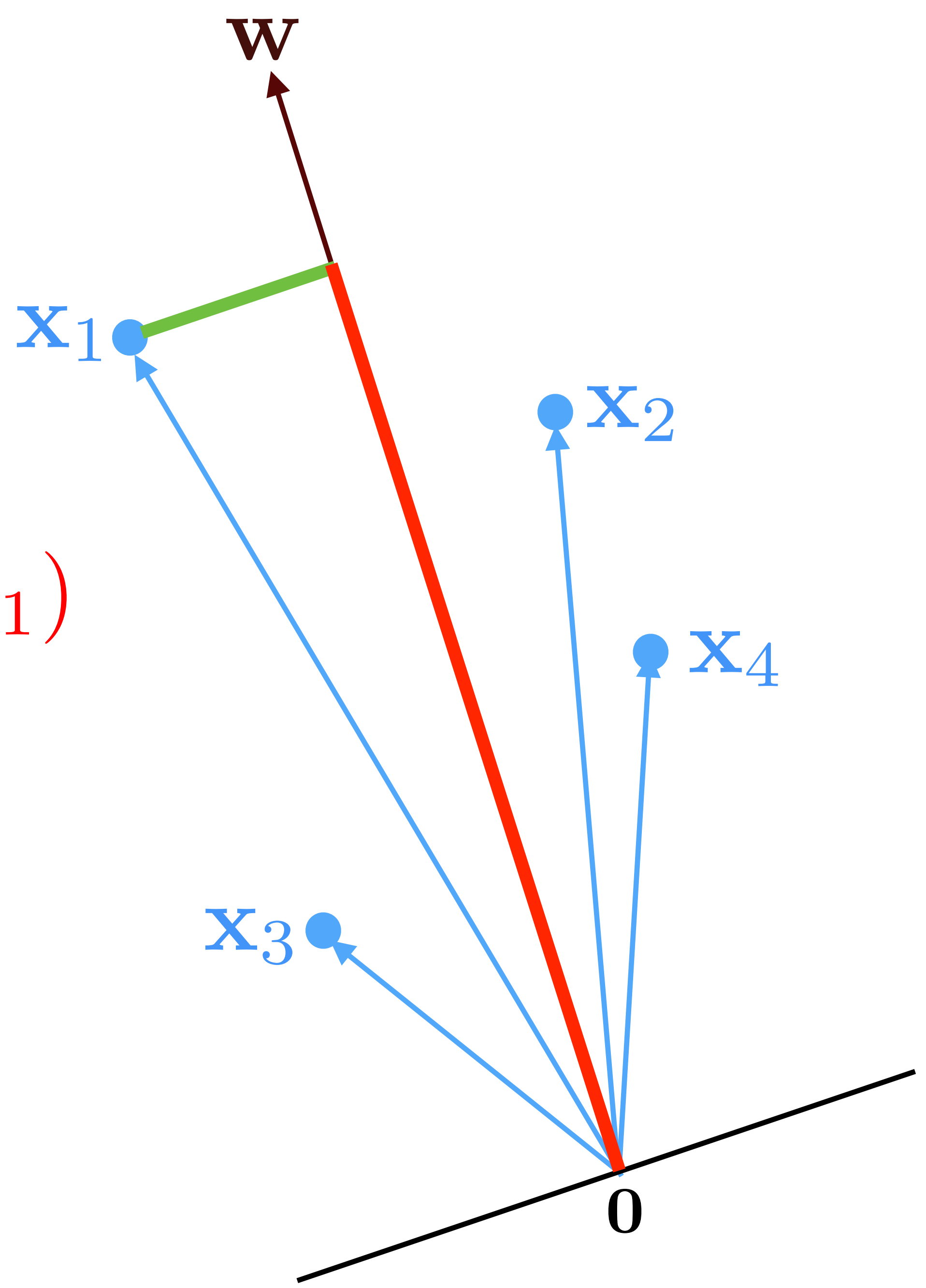


Prelude: reducing to 1 dimension

$$\mathbf{y}_1 = \mathbf{w}^\top \mathbf{x}_1 = \|\mathbf{x}_1\| \cos\left(\angle \mathbf{w}\mathbf{x}_1\right)$$

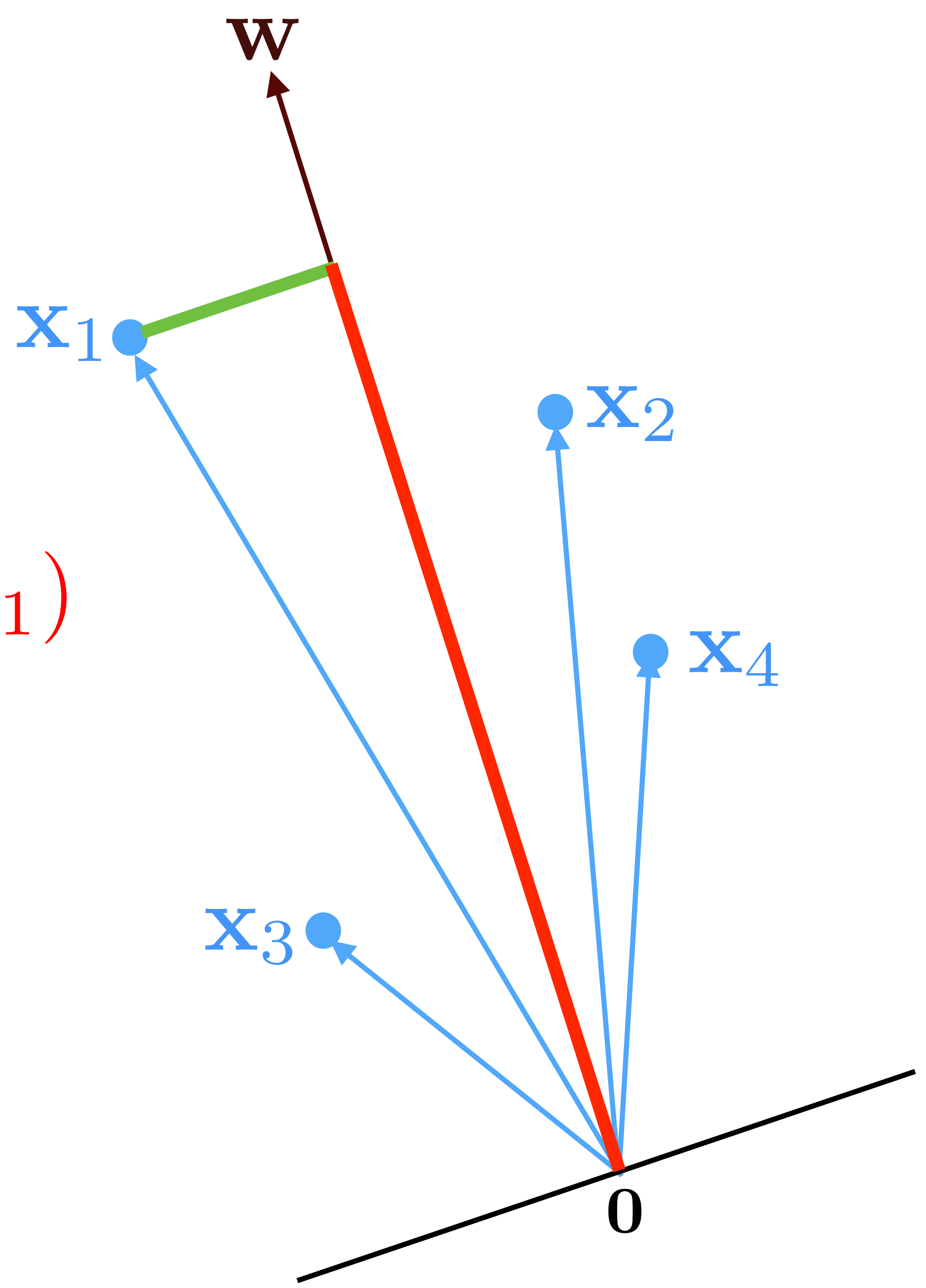


Dim Reduction: Linear Transformation

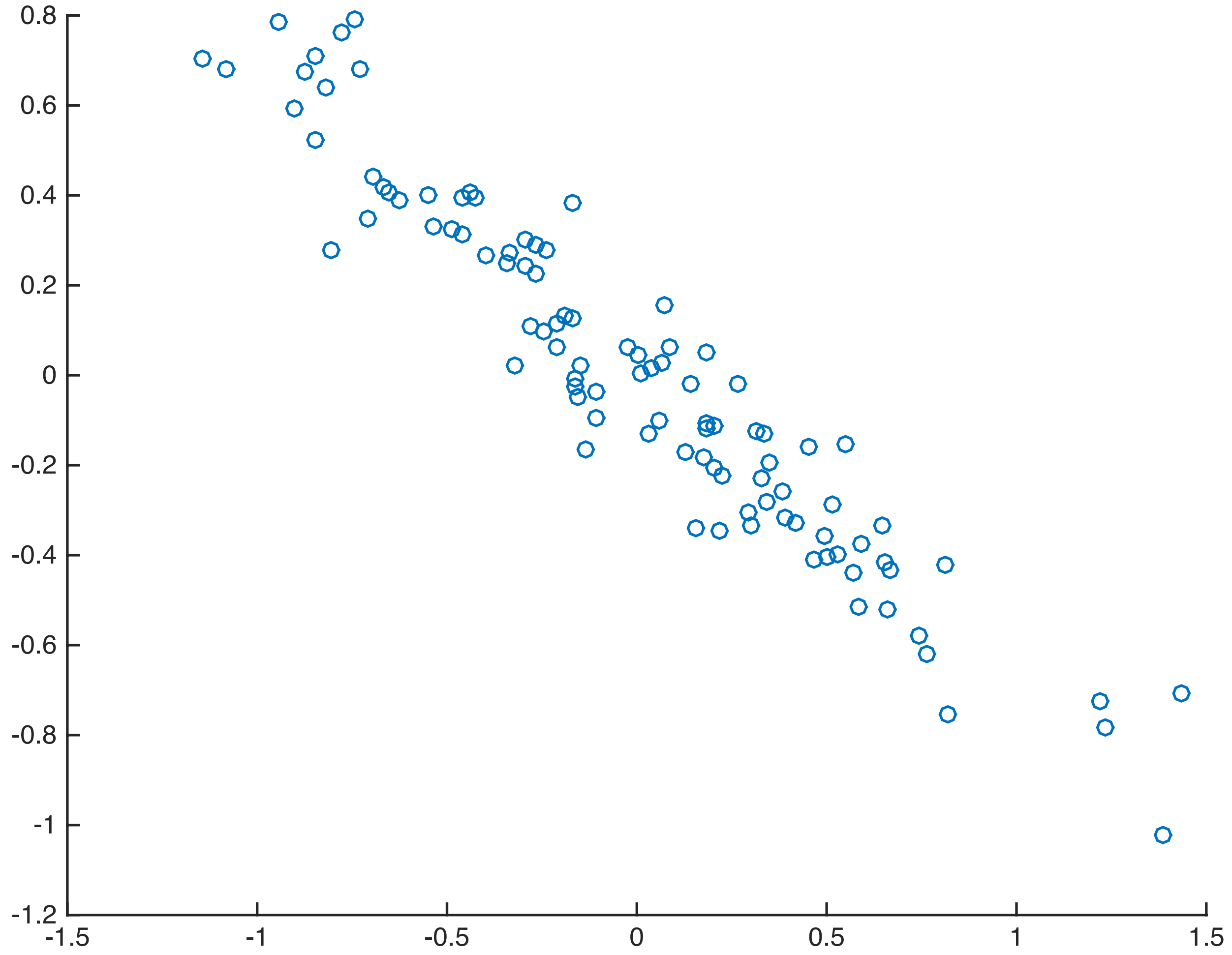
Prelude: reducing to 1 dimension

$$\mathbf{y}_1 = \mathbf{w}^\top \mathbf{x}_1 = \|\mathbf{x}_1\| \cos\left(\angle \mathbf{w}\mathbf{x}_1\right)$$

Only direction matters, assume without loss of generality that ||w|| = 1



PCA: Variance Maximization



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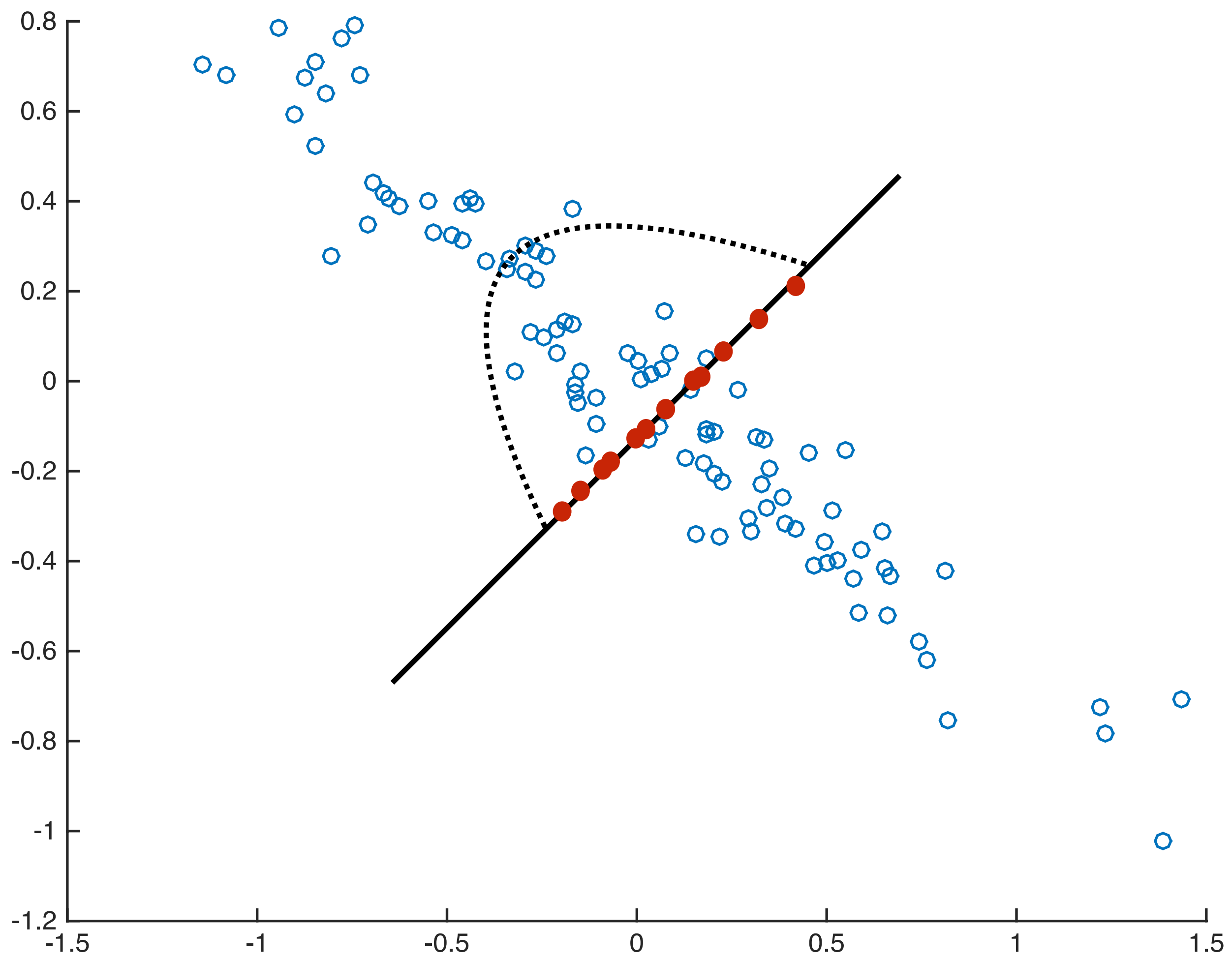

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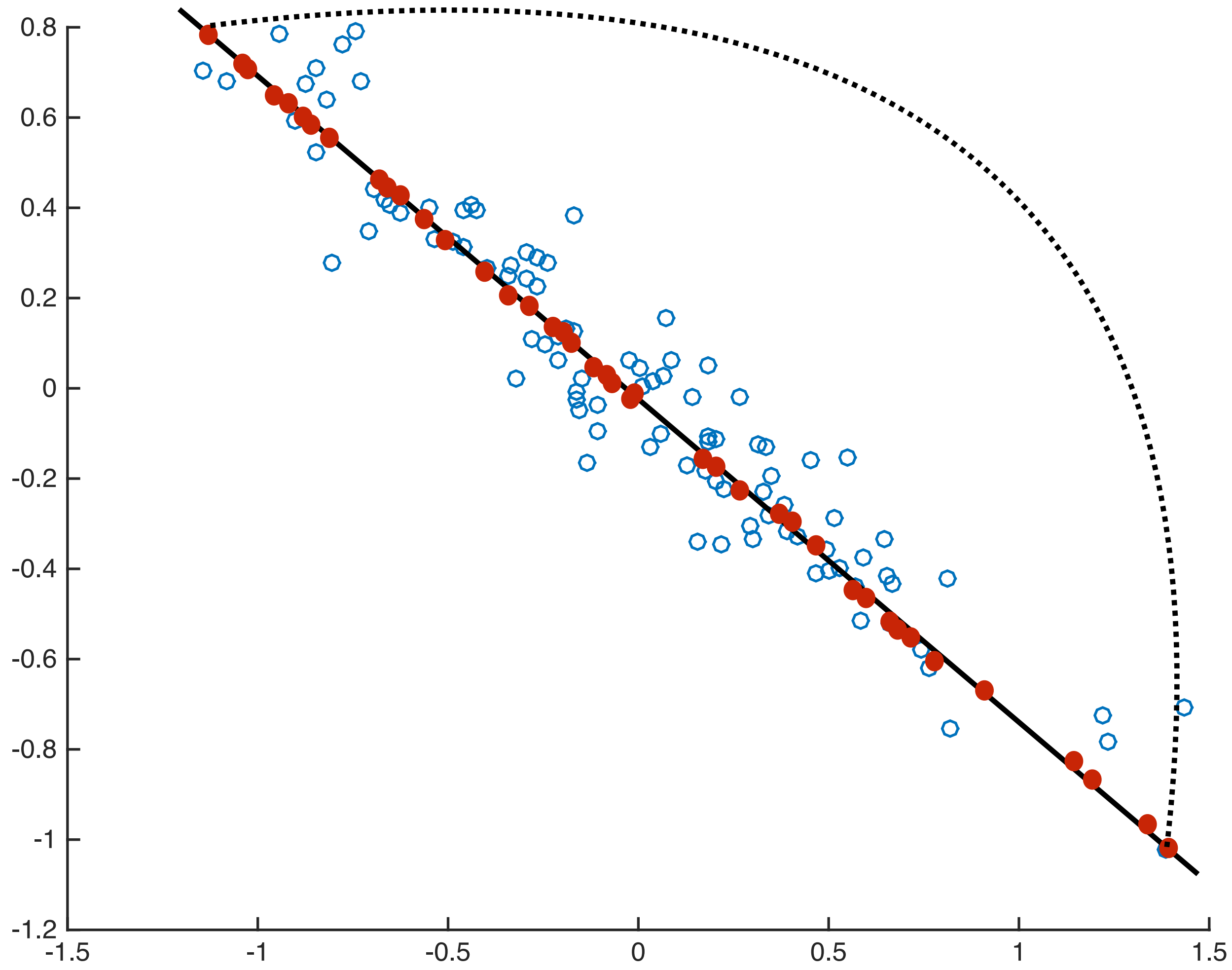

PCA: Variance Maximization

- Pick directions along which data varies the most

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$$\text{Variance} = \frac{1}{n}\sum_{t=1}^{n}\left(y_t - \frac{1}{n}\sum_{s=1}^{n} y_s\right)^2$$

PCA: Variance Maximization

- Pick directions along which data varies the most

$$\text{Variance} = \frac{1}{n}\sum_{t=1}^{n}\left(y_t - \frac{1}{n}\sum_{s=1}^{n} y_s\right)^2$$

$$= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top \mathbf{x}_t - \frac{1}{n}\sum_{s=1}^{n} \mathbf{w}^\top \mathbf{x}_s\right)^2$$

PCA: Variance Maximization

- Pick directions along which data varies the most

$$
\begin{aligned}
\text{Variance} &= \frac{1}{n}\sum_{t=1}^{n}\left(y_t - \frac{1}{n}\sum_{s=1}^{n} y_s\right)^2 \\
&= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top \mathbf{x}_t - \frac{1}{n}\sum_{s=1}^{n} \mathbf{w}^\top \mathbf{x}_s\right)^2 \\
&= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top \mathbf{x}_t - \mathbf{w}^\top\left(\frac{1}{n}\sum_{s=1}^{n} \mathbf{x}_s\right)\right)^2
\end{aligned}
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&= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top (\mathbf{x}_t - \mu)\right)^2
\end{aligned}
$$

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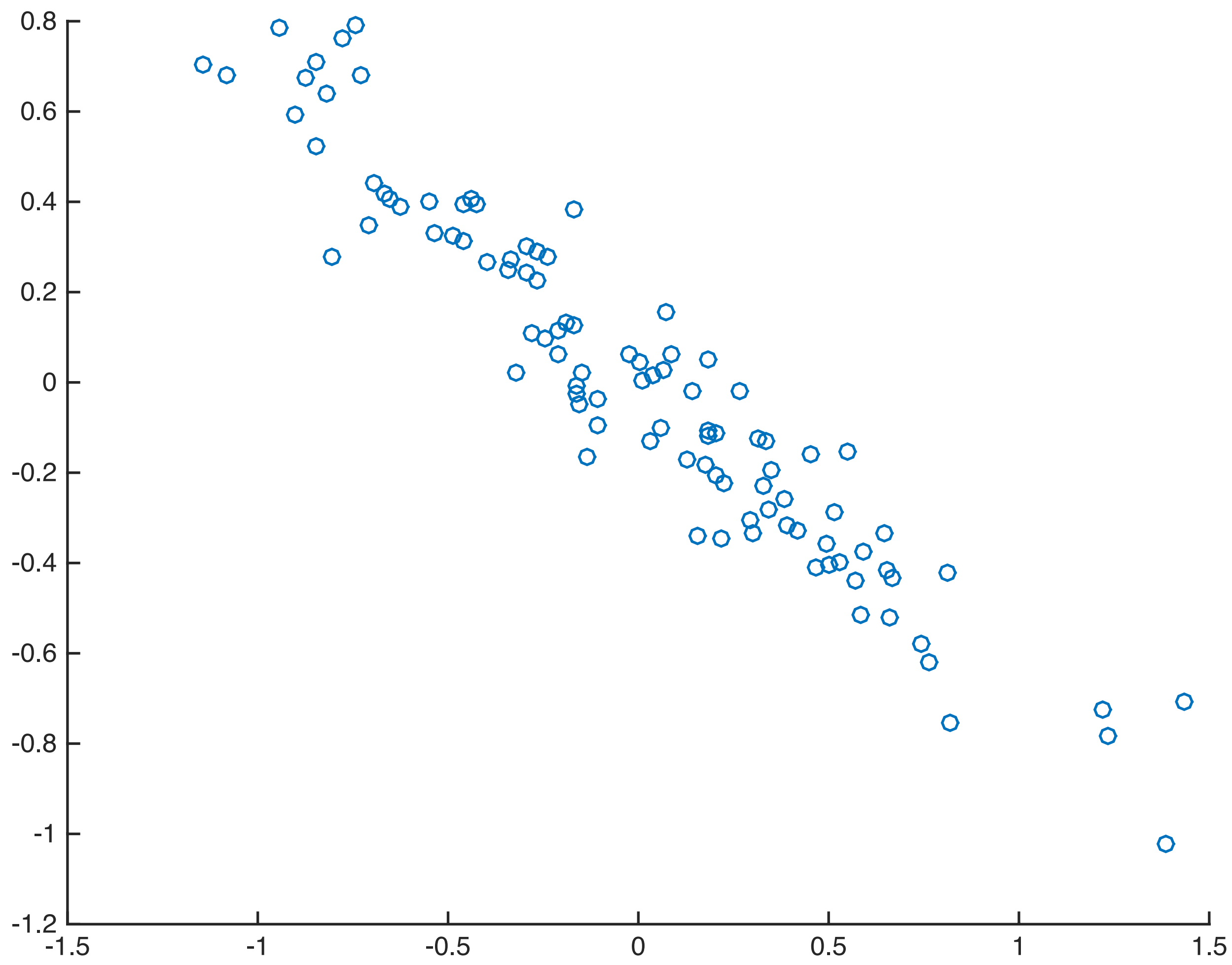
&= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top(\mathbf{x}_t - \mu)\right)^2 \\
&= \text{ average squared inner product}
\end{aligned}
$$

Which Direction?



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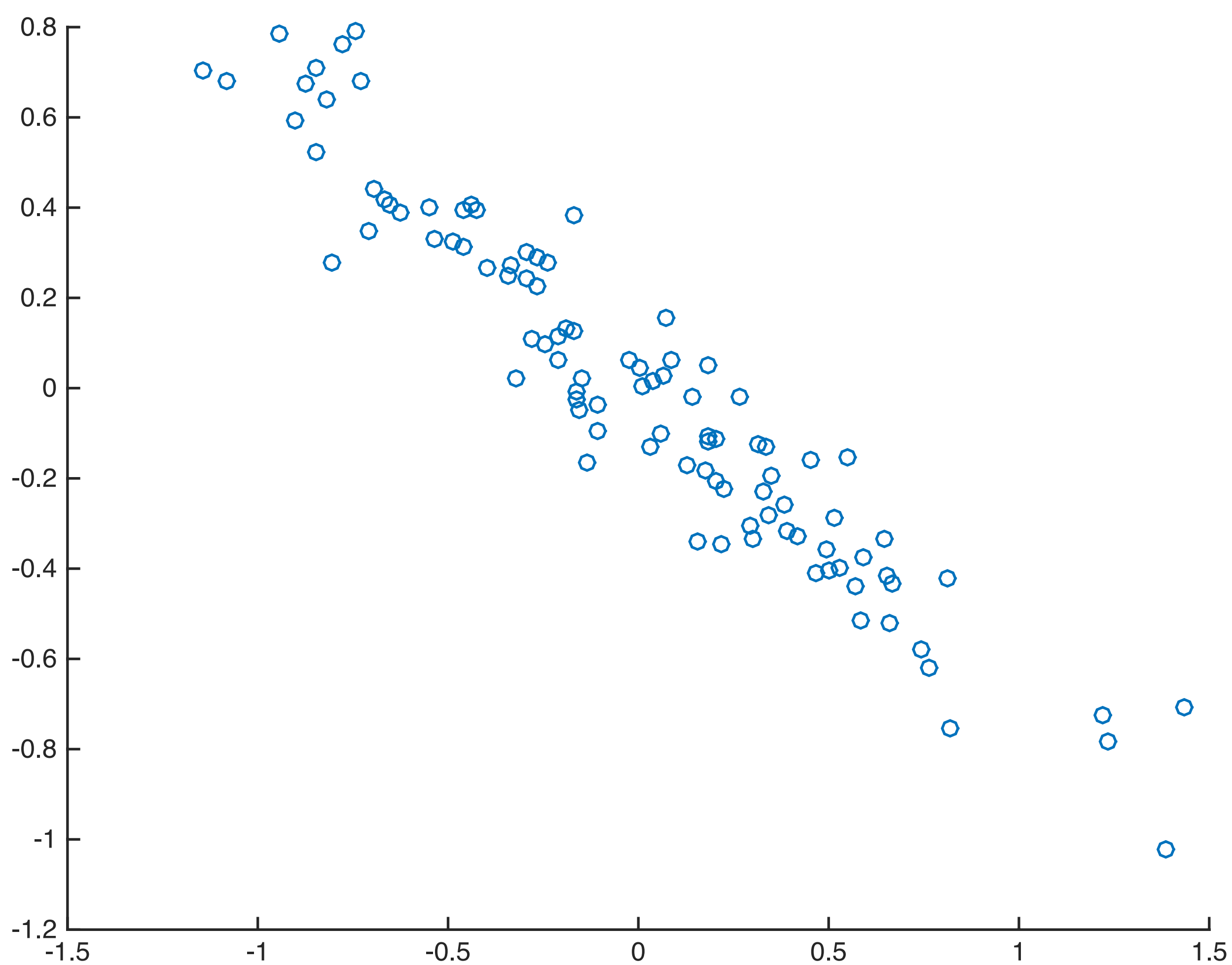

$$\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top(\mathbf{x}_t-\mu)\right)^2 = \frac{1}{n}\sum_{t=1}^{n}\|\mathbf{x}_t-\mu\|^2\text{cosine}(w, x_t-\mu)$$

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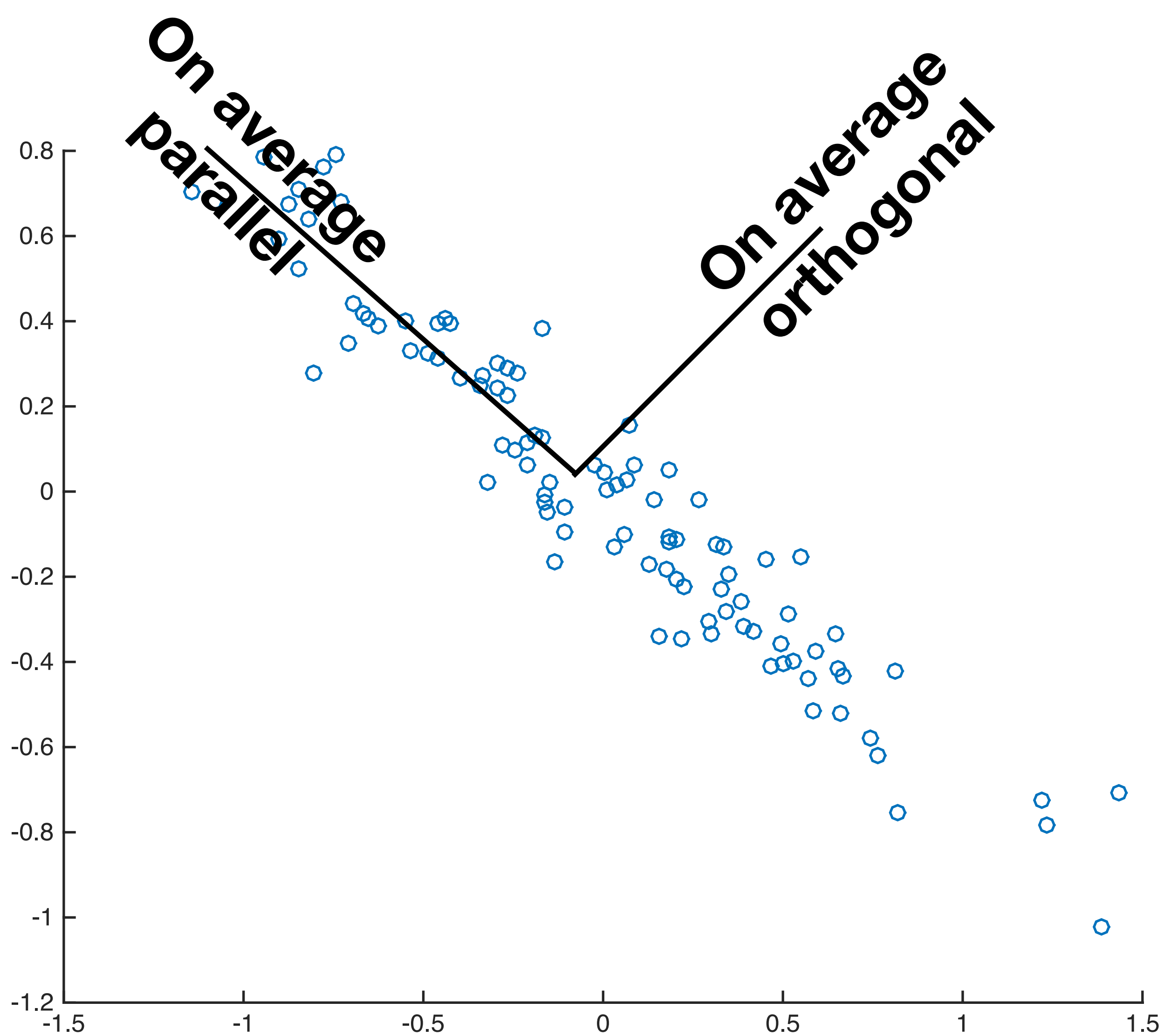

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PCA: Variance Maximization

- Pick directions along which data varies the most
- First principal component:

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

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

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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}
\end{aligned}$$

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&= \arg\max_{\mathbf{w}:\|\mathbf{w}\|_2=1} \mathbf{w}^\top \Sigma \mathbf{w}
\end{aligned}$$

Σ is the covariance matrix

Covariance Matrix

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

$$\Sigma[i,j] = \frac{1}{n}\sum_{t=1}^{n}(\mathbf{x}_t[i] - \mu[i])(\mathbf{x}_t[j] - \mu[j])$$

PCA: Variance Maximization

Covariance matrix:

$$\Sigma = \frac{1}{n}\sum_{t=1}^{n}(\mathbf{x}_t - \mu)(\mathbf{x}_t - \mu)^\top$$

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PCA: Variance Maximization

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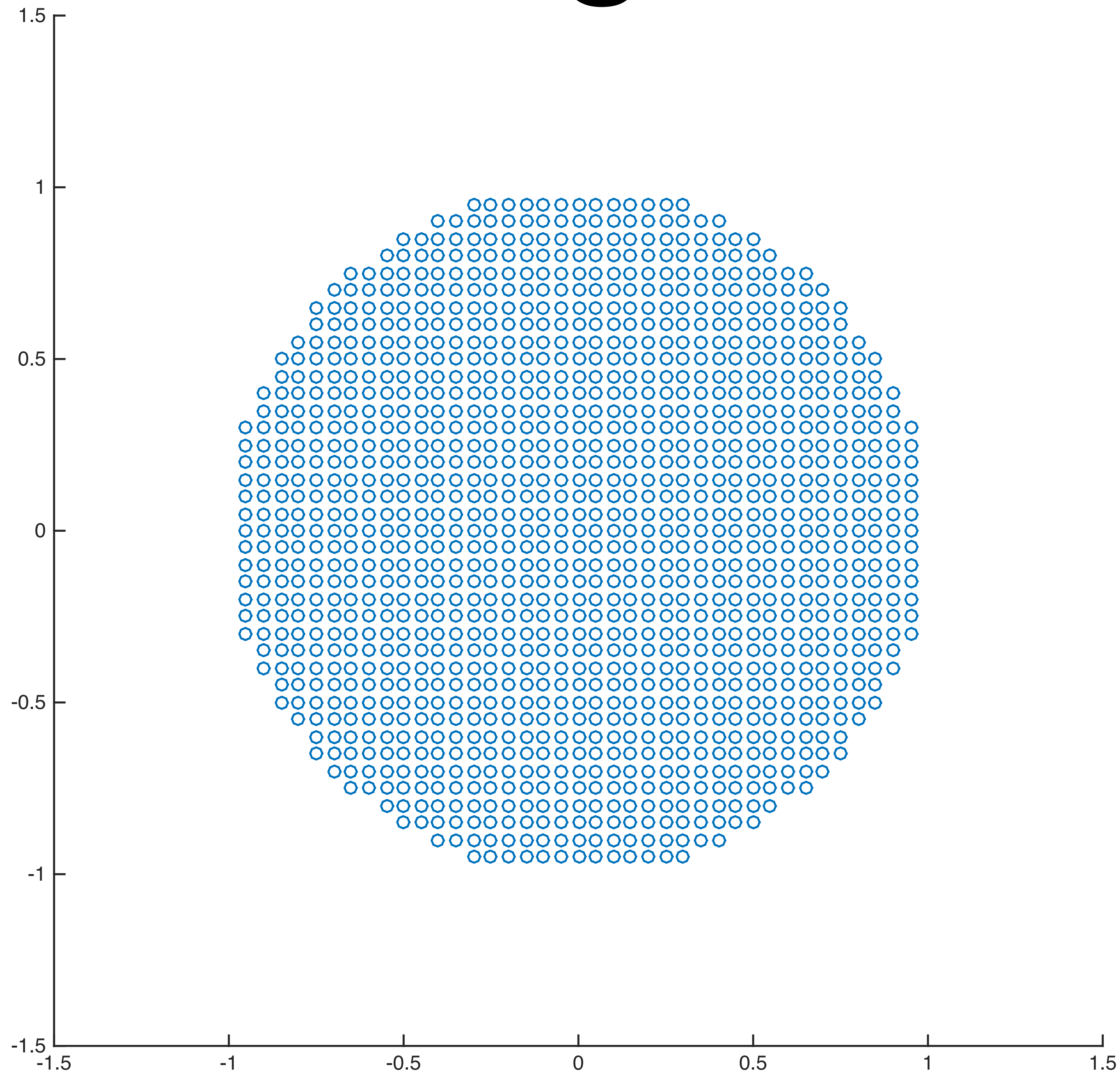
Σ is the covariance matrix

Solution: $\mathbf{w}_1 =$ Largest Eigenvector of Σ

What are Eigen Vectors?



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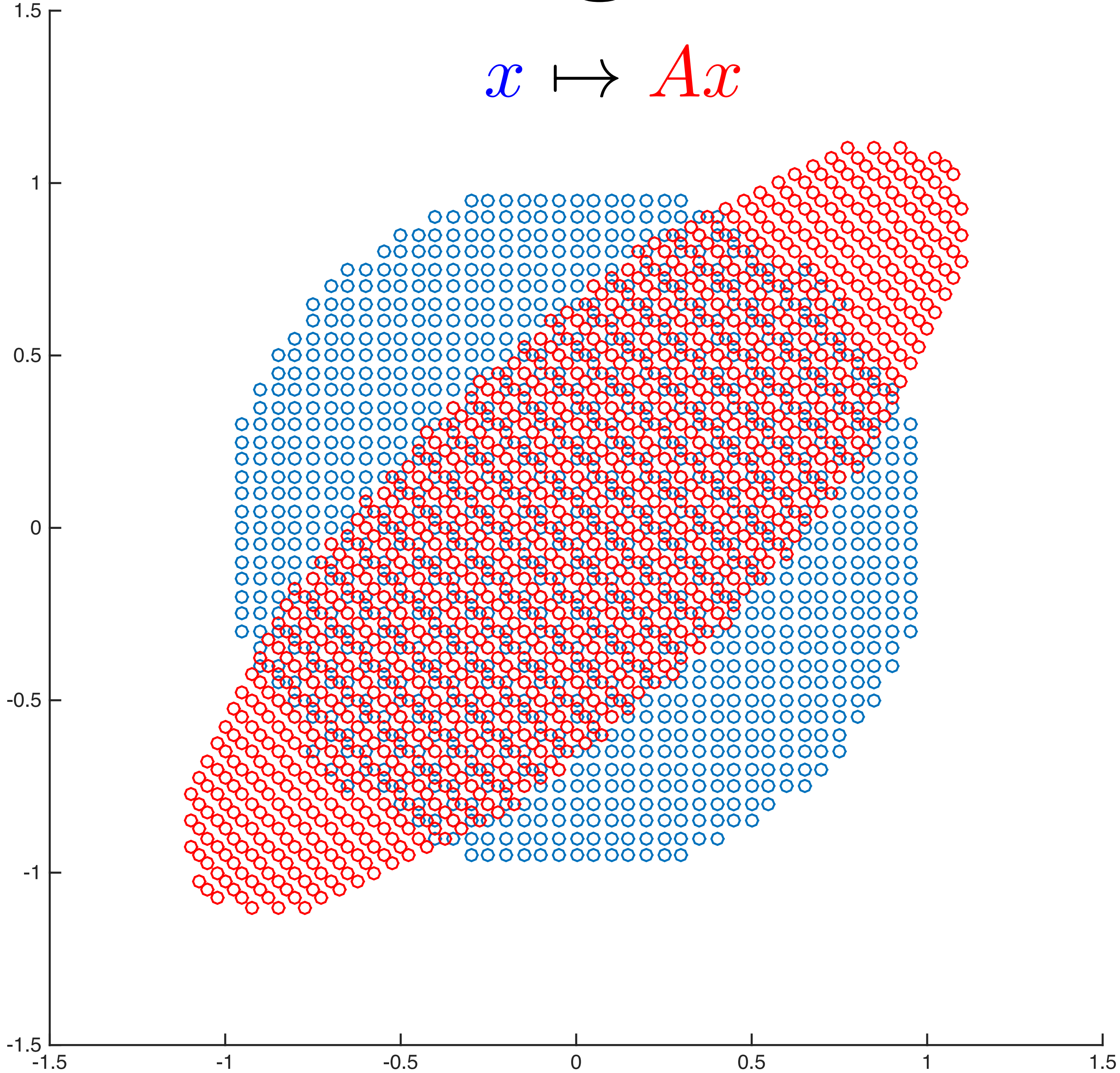

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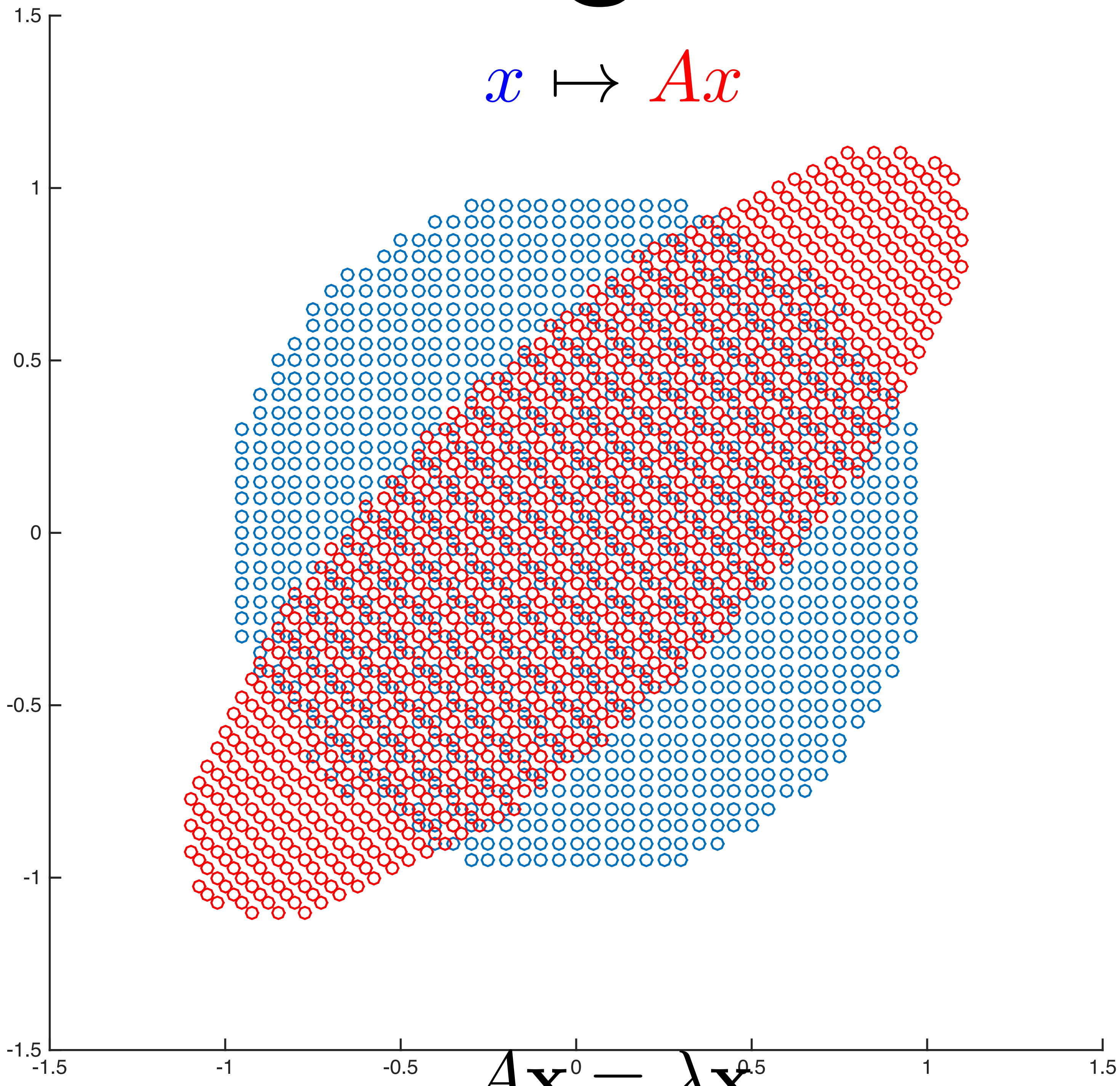

$$A\mathbf{x} = \lambda\mathbf{x}$$

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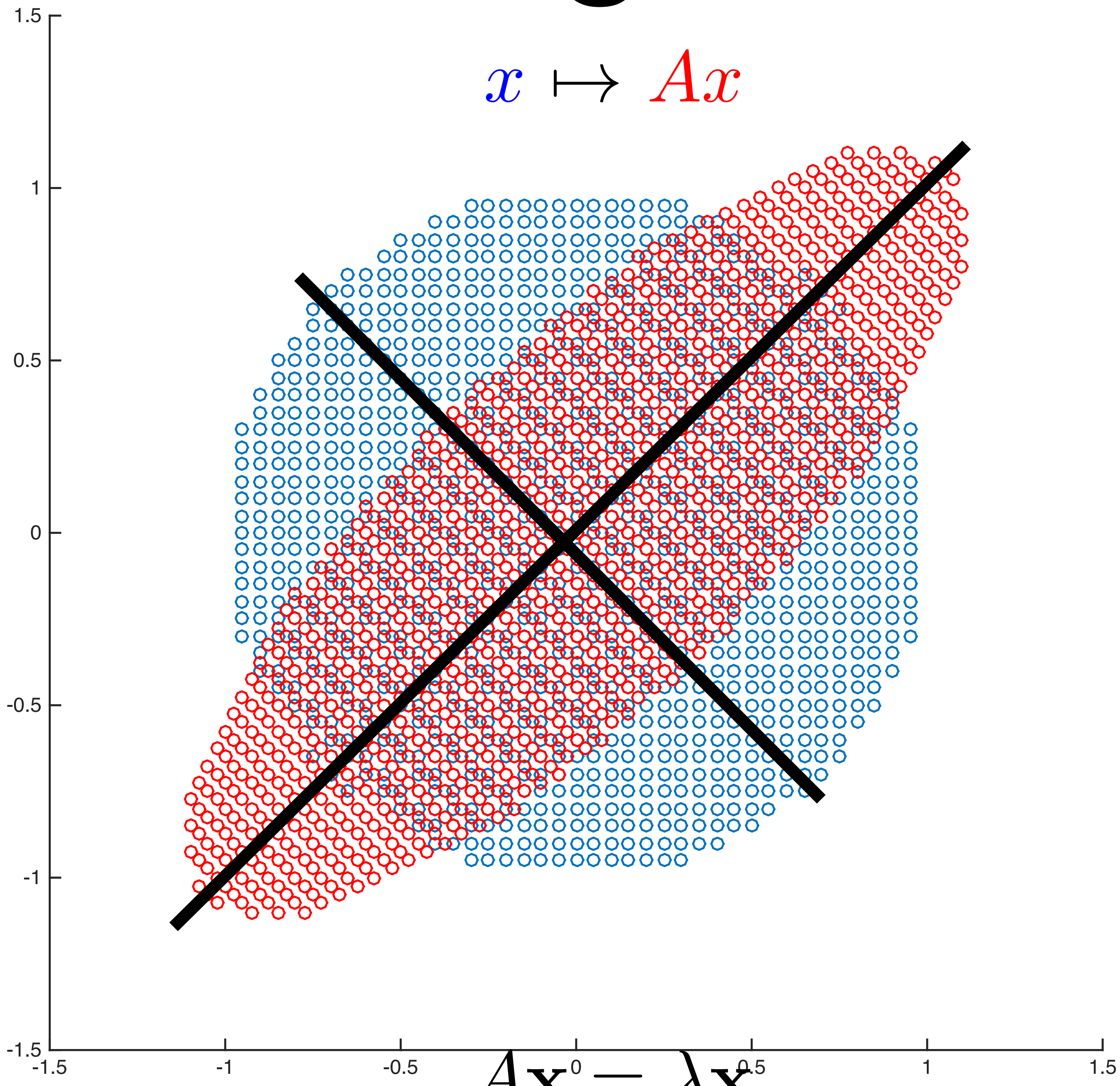

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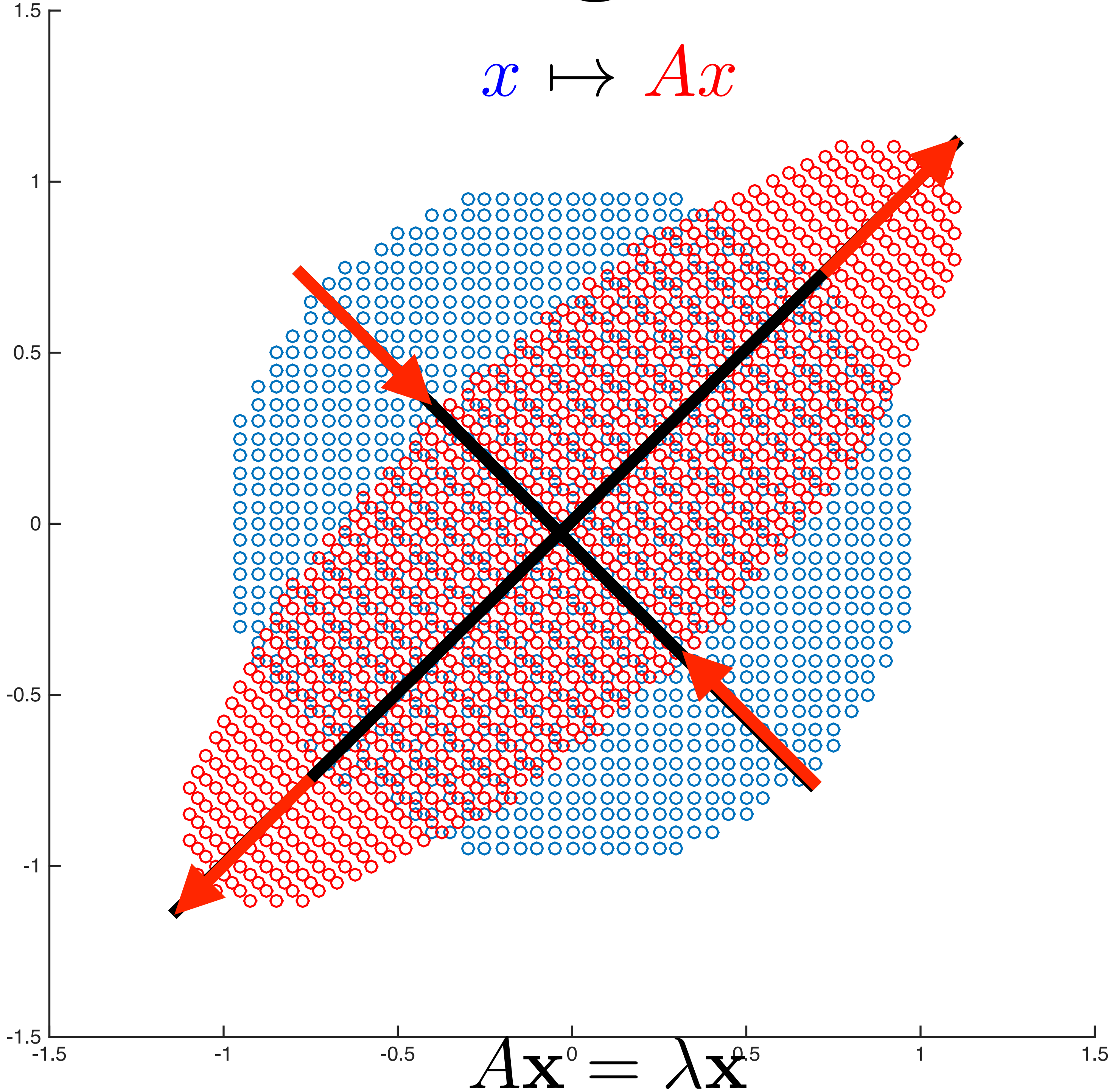

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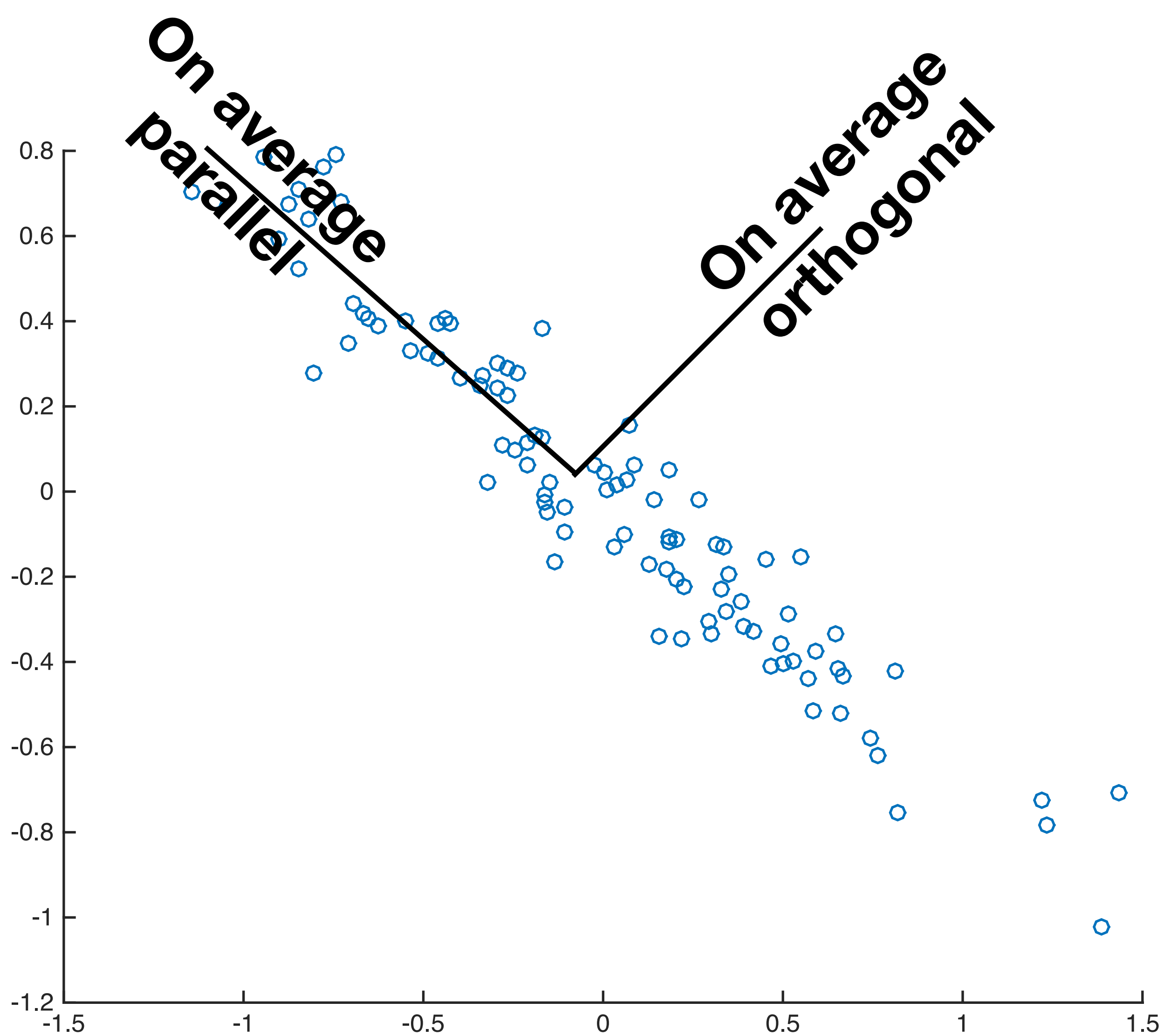

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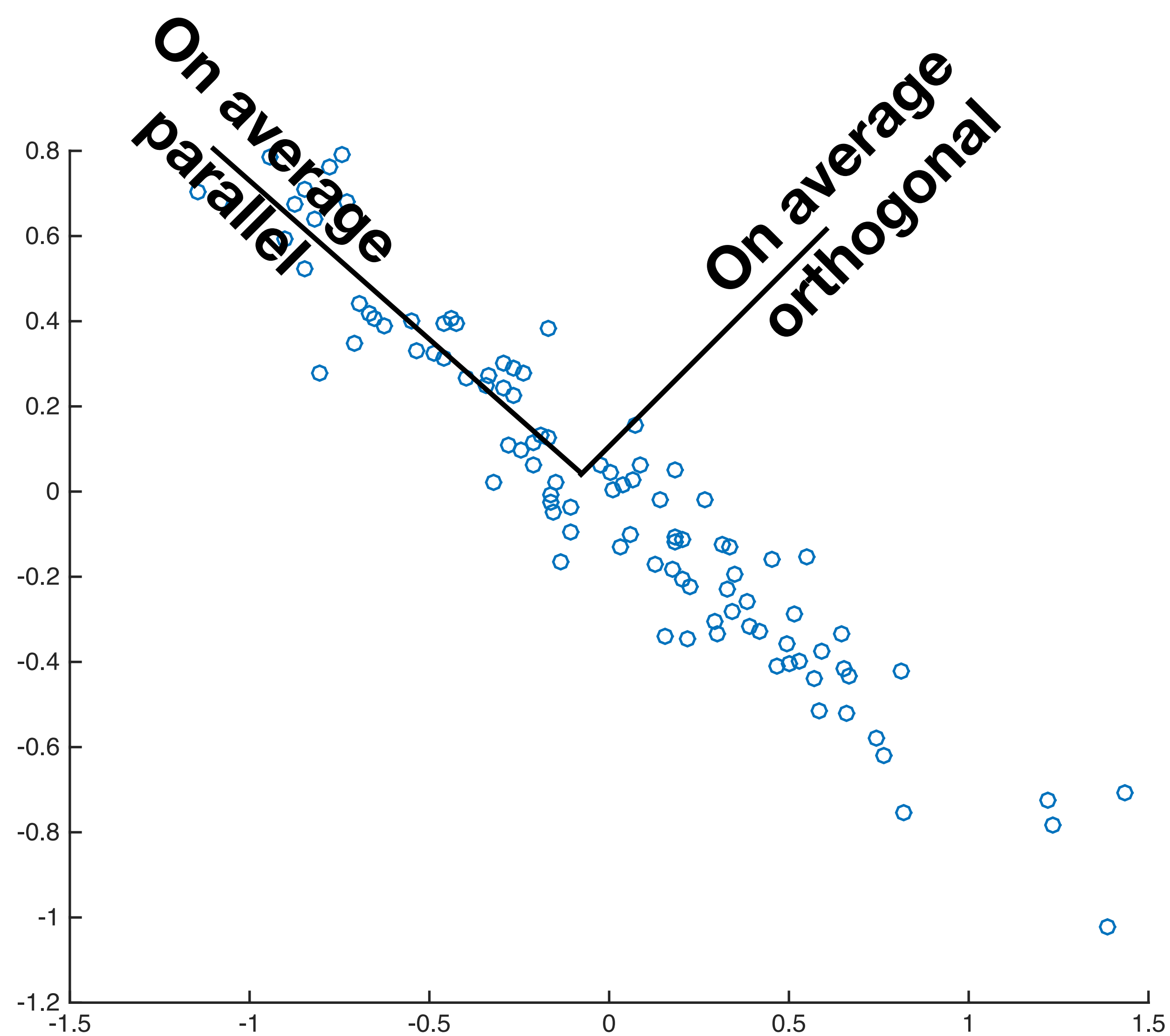


Top Eigenvector of covariance matrix

- What if we want more than one number for each data point?
- That is we want to reduce to K > 1 dimensions?

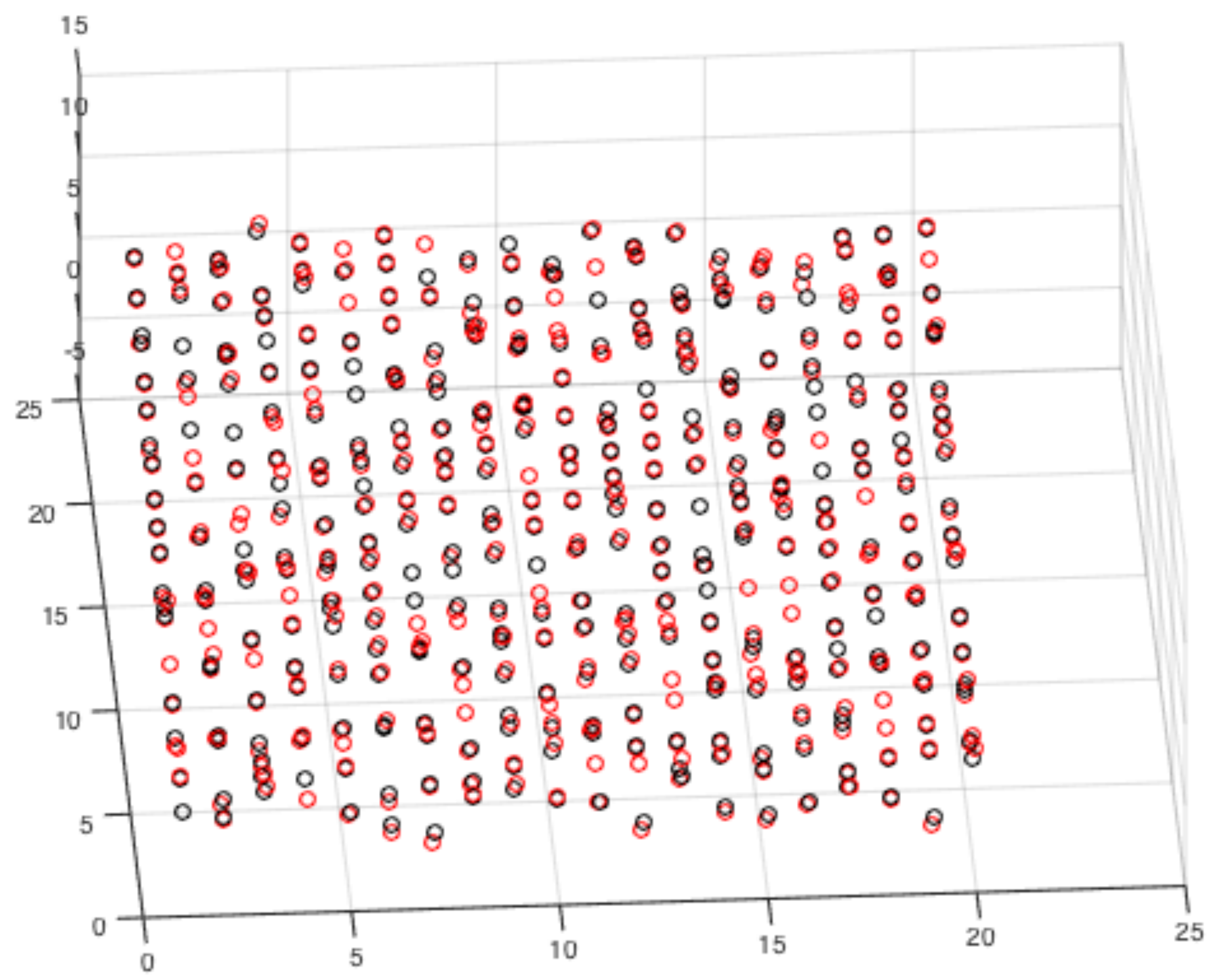
PCA: Variance Maximization

- How do we find the K components?

PCA: Variance Maximization

- How do we find the K components?

Ans: Maximize sum of spread in the K directions



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Intuition: Remove top direction, now reduce dimension for remaining d-1 dimensions

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Principal Component Analysis

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

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

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

Can we reconstruct the original data points?