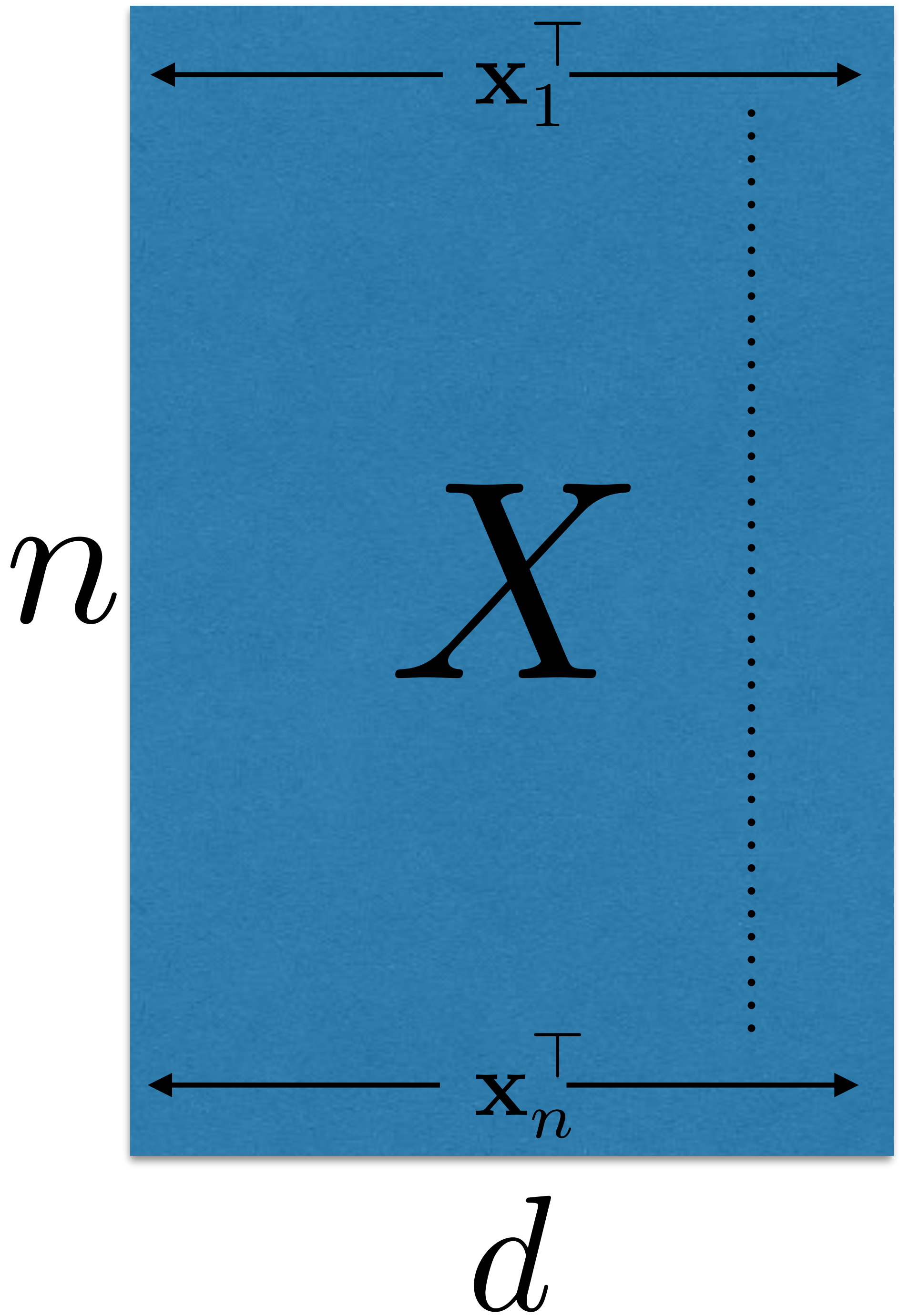
Machine Learning for Data Science (CS4786)
Lecture 3

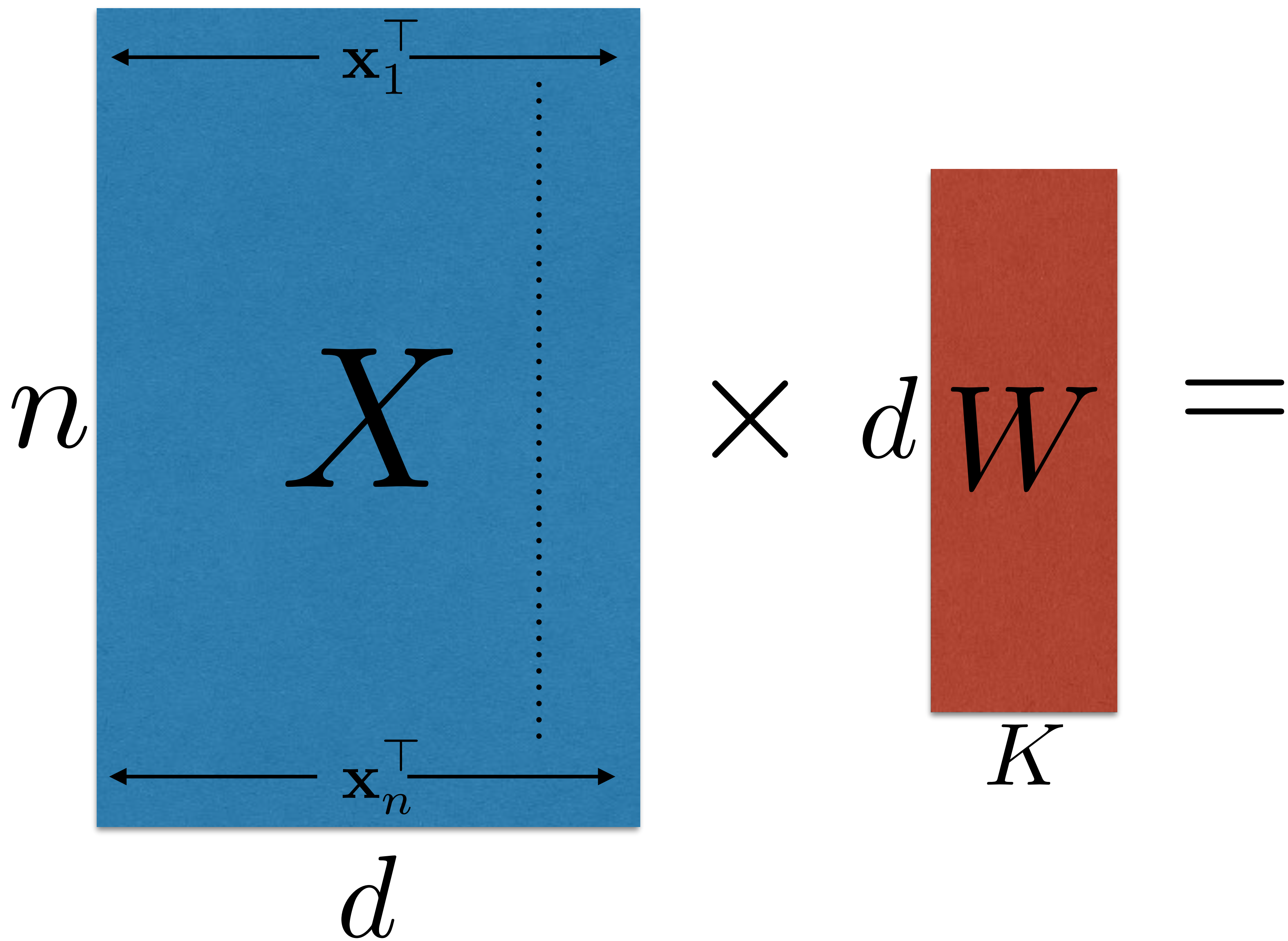
Principal Component Analysis

Dim Reduction: Linear Transformation

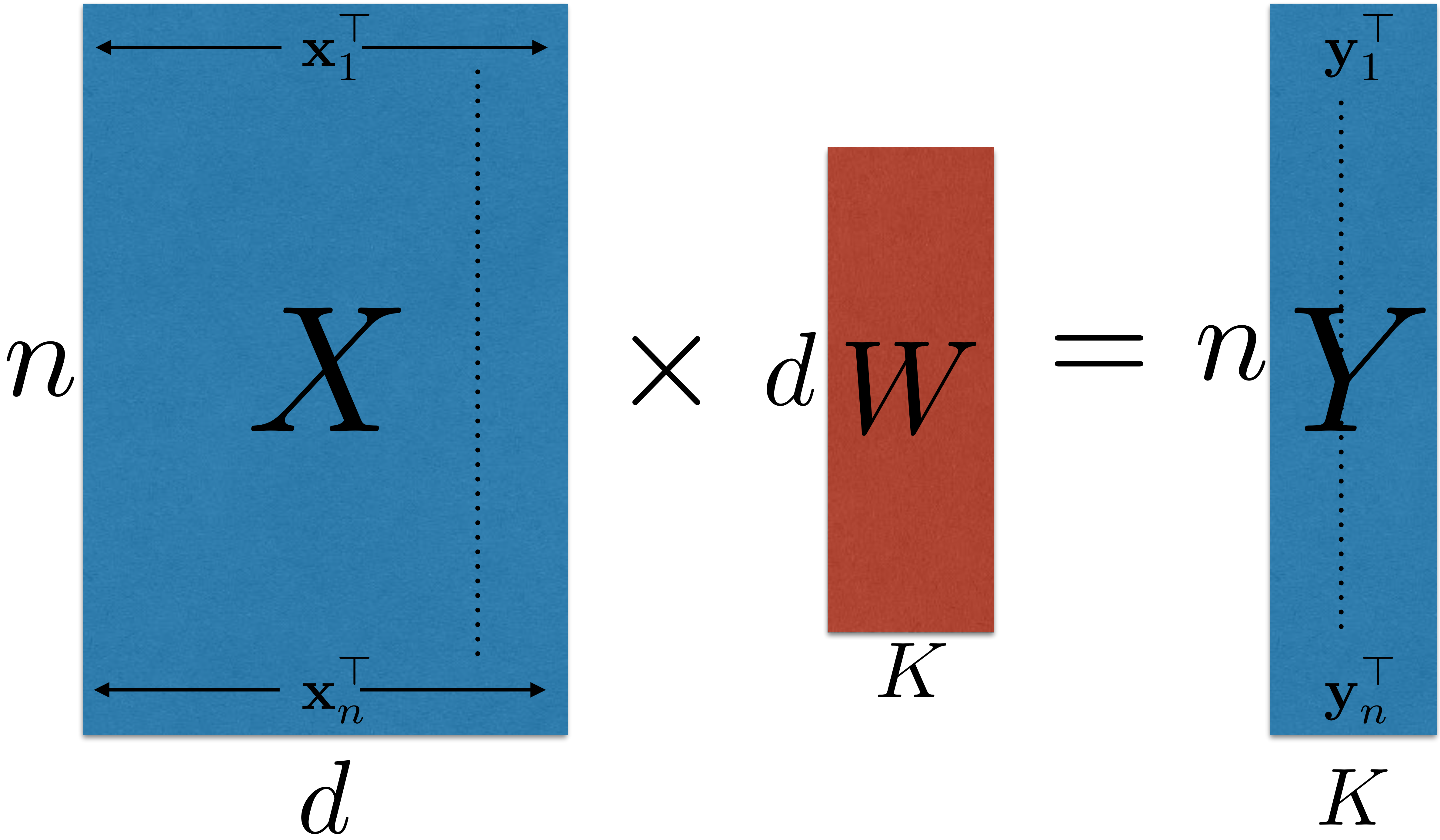
Dim Reduction: Linear Transformation



DIM REDUCTION: LINEAR TRANSFORMATION



Dim Reduction: Linear Transformation



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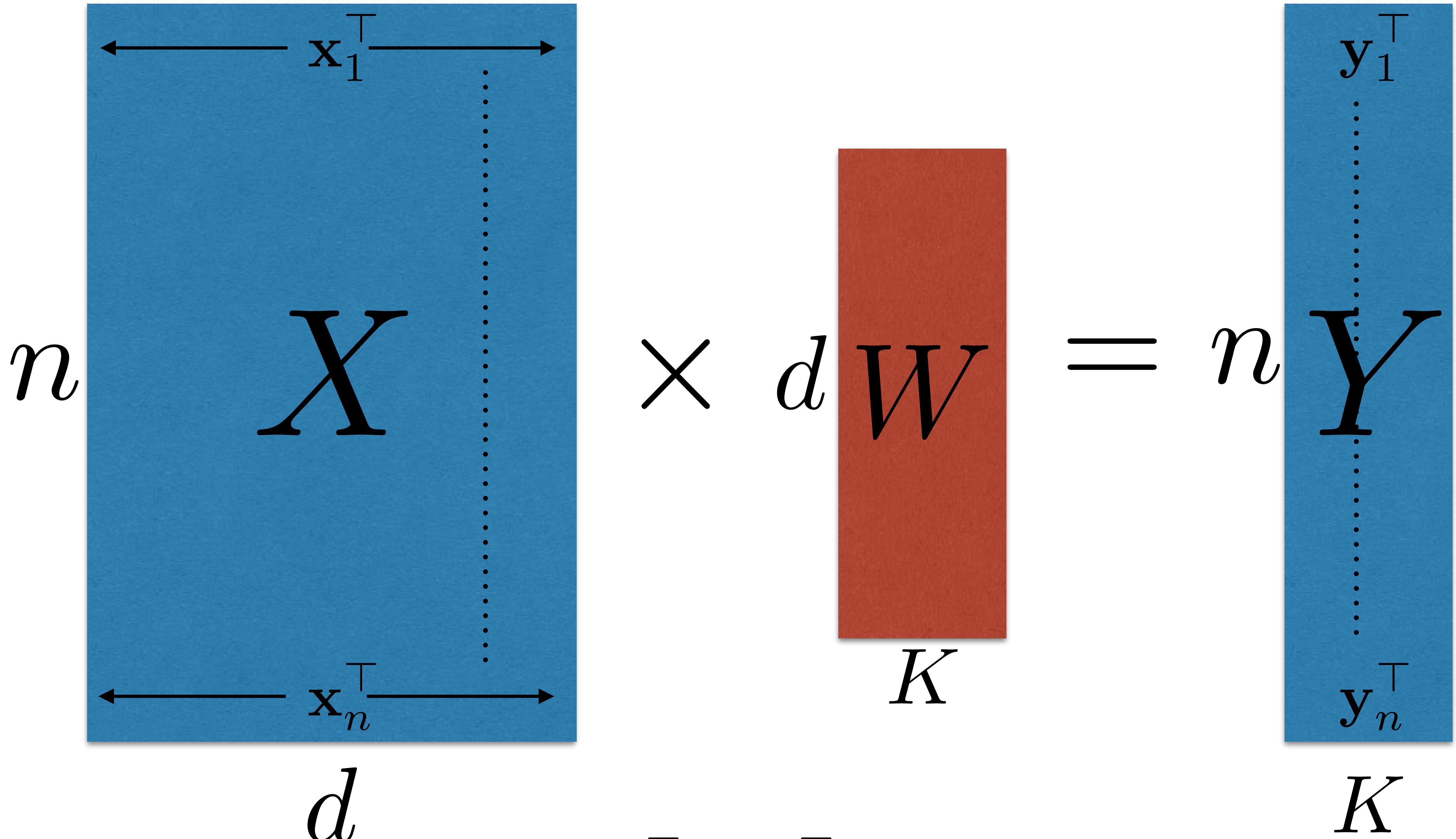
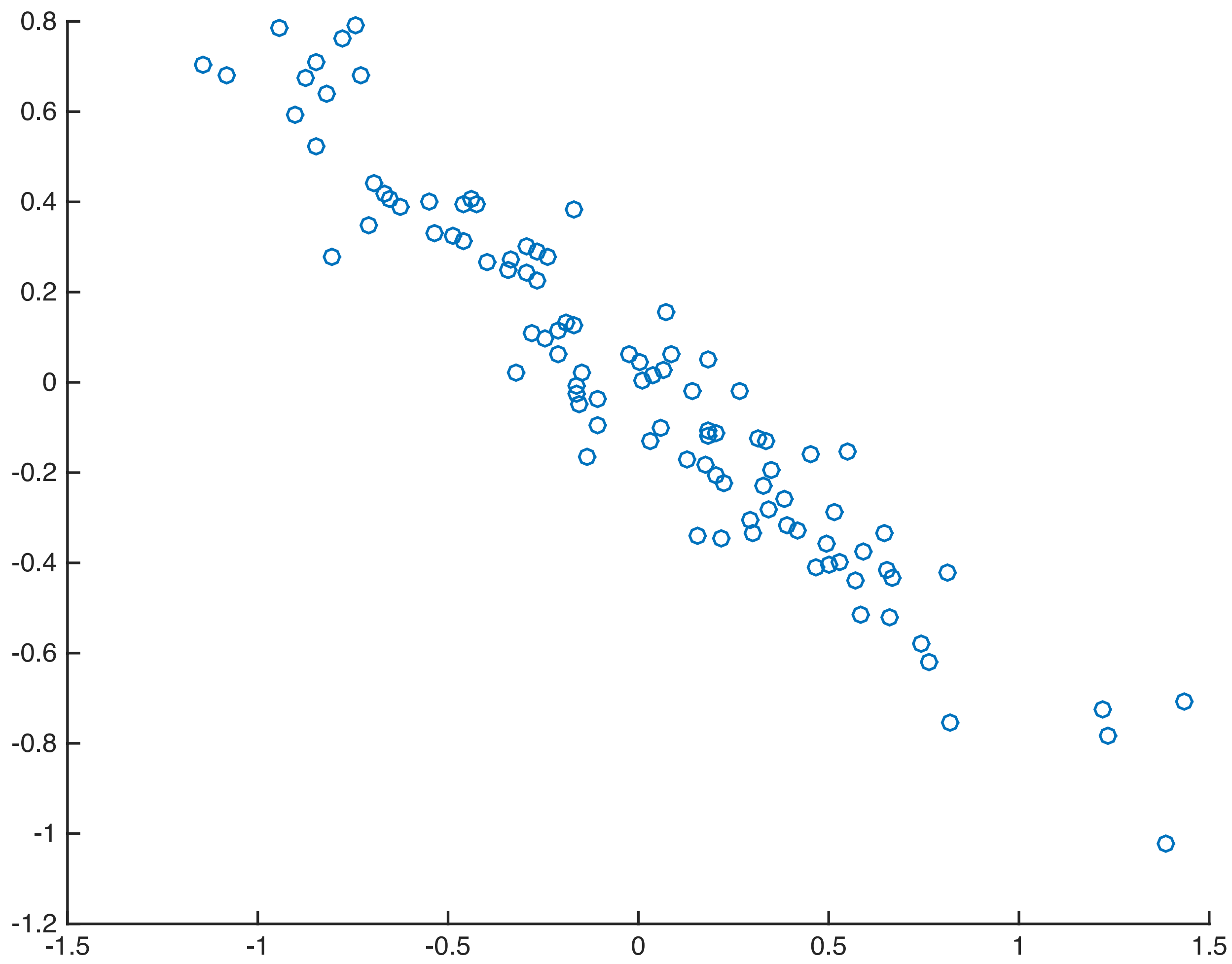


$$\mathbf{y}_i^\top = \mathbf{x}_i^\top W$$

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?

PCA: Variance Maximization



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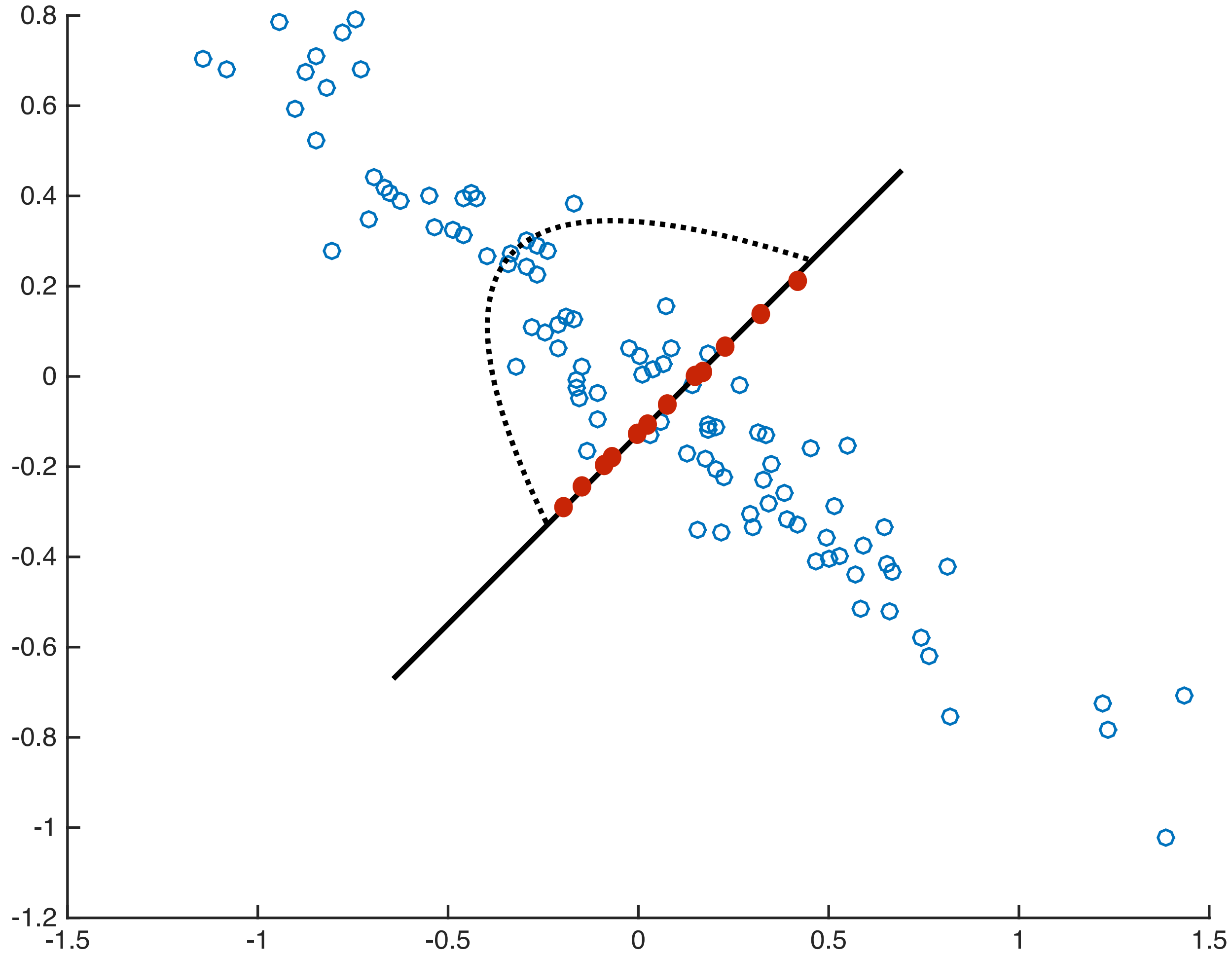

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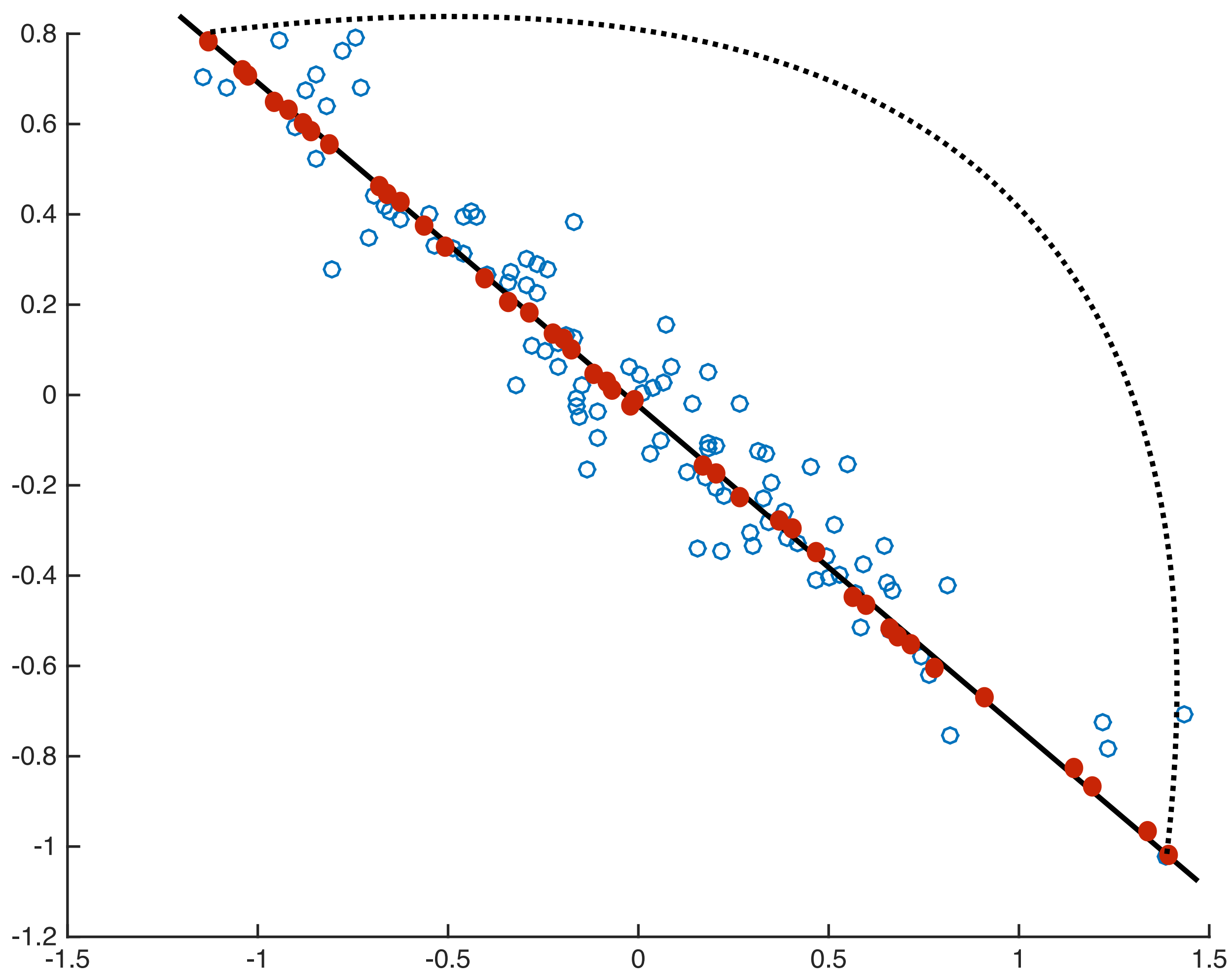

PCA: Variance Maximization

- Pick directions along which data varies the most

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

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

PCA: Variance Maximization

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

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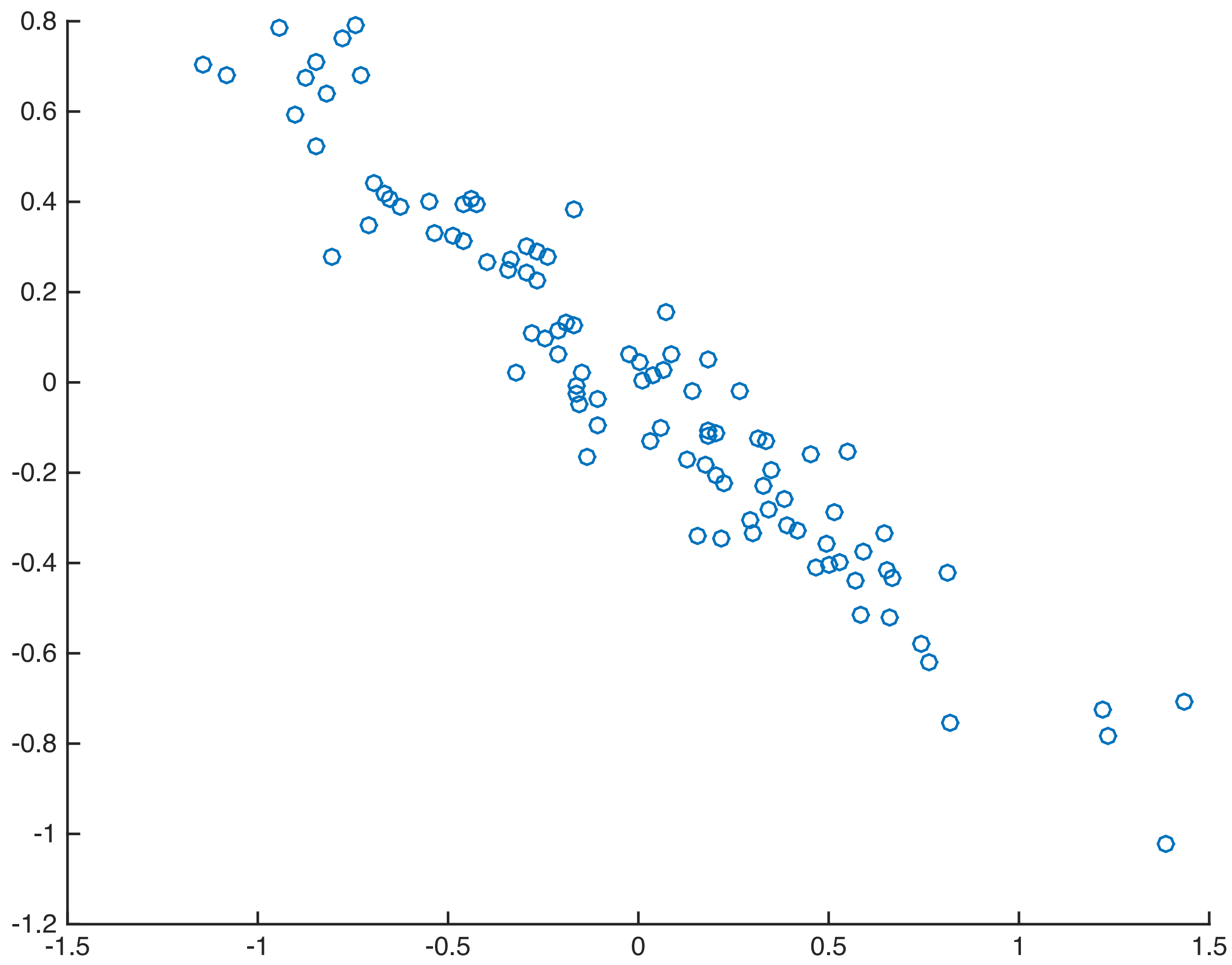
&= \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top (\mathbf{x}_t - \mu)\right)^2 \\
&= \text{ average squared inner product}
\end{aligned}
$$

Which Direction?



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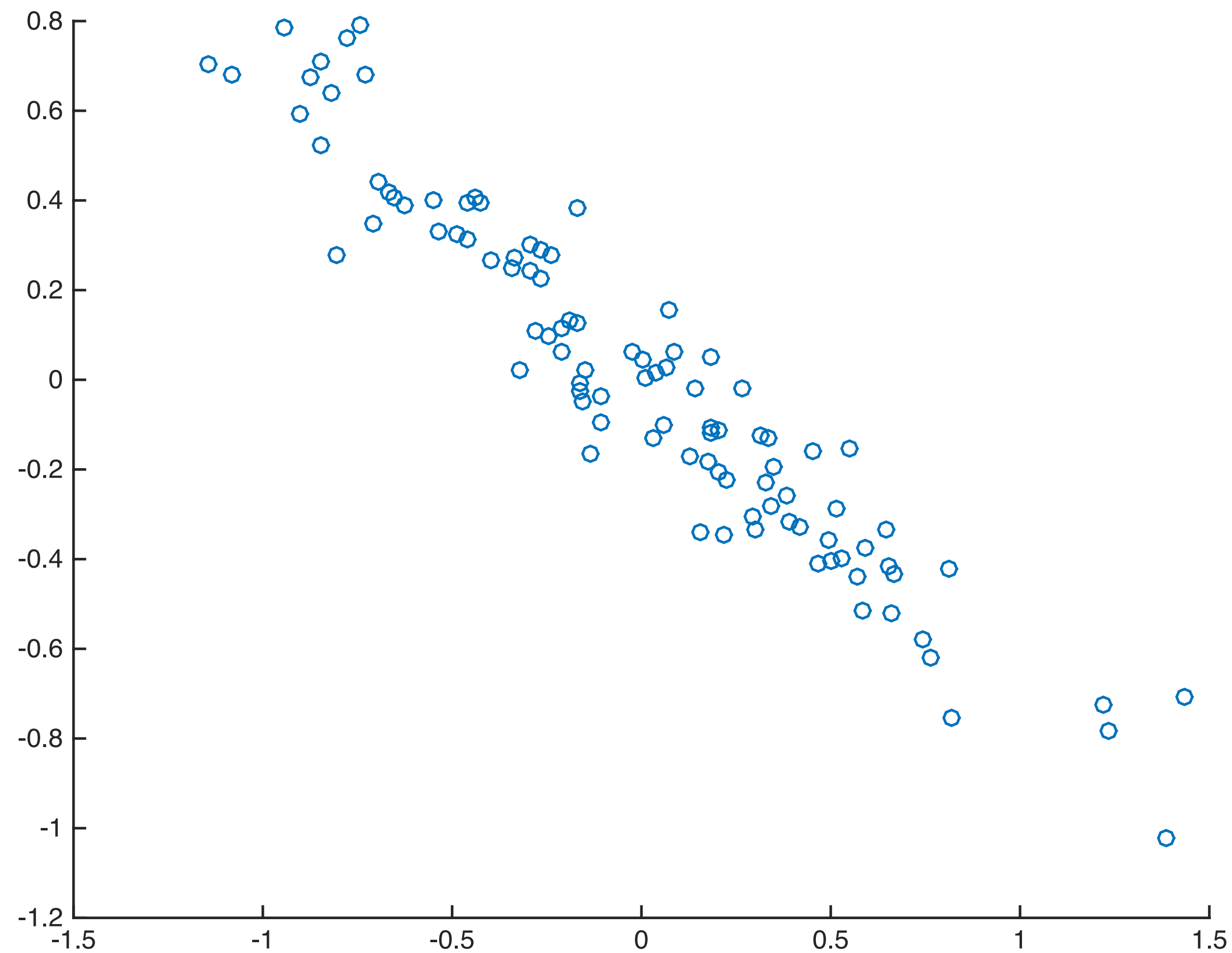

$$\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{w}^\top(\mathbf{x}_t-\mu)\right)^2 = \frac{1}{n}\sum_{t=1}^{n}\|\mathbf{x}_t-\mu\|^2 \text{cosine}(w, x_t-\mu)$$

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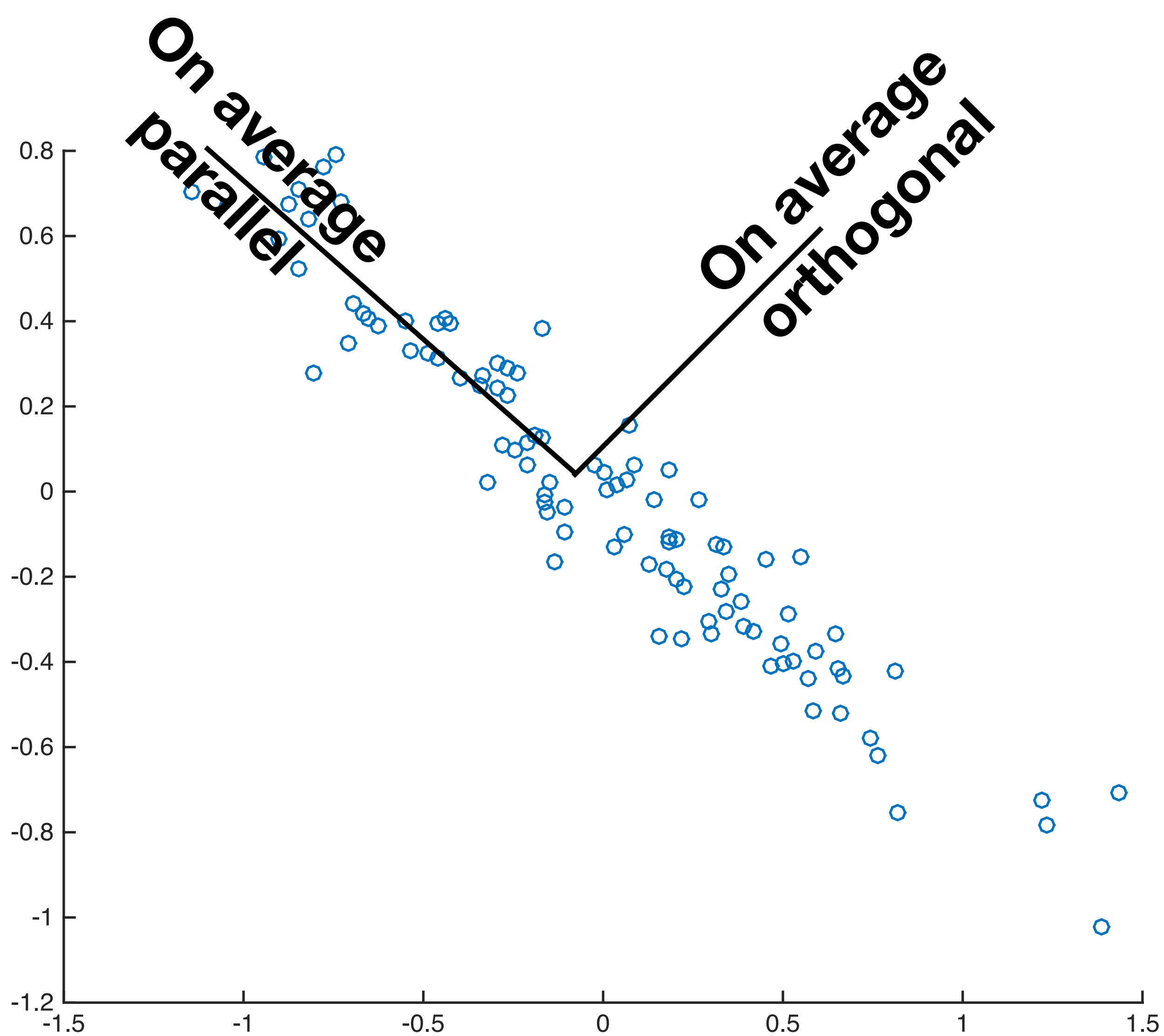

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PCA: Variance Maximization

- 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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Σ is the covariance matrix

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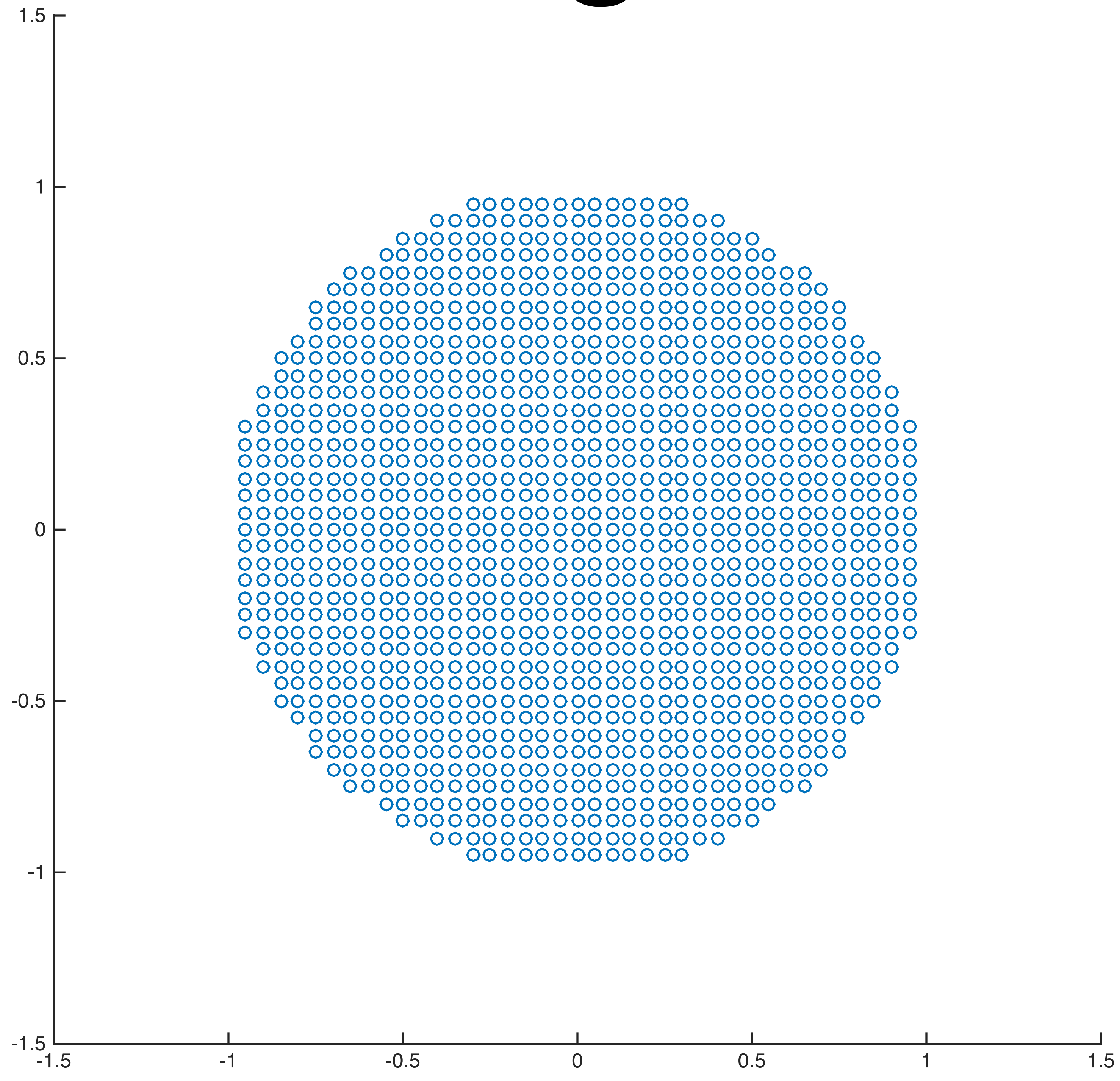
Σ is the covariance matrix

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

What are Eigen Vectors?



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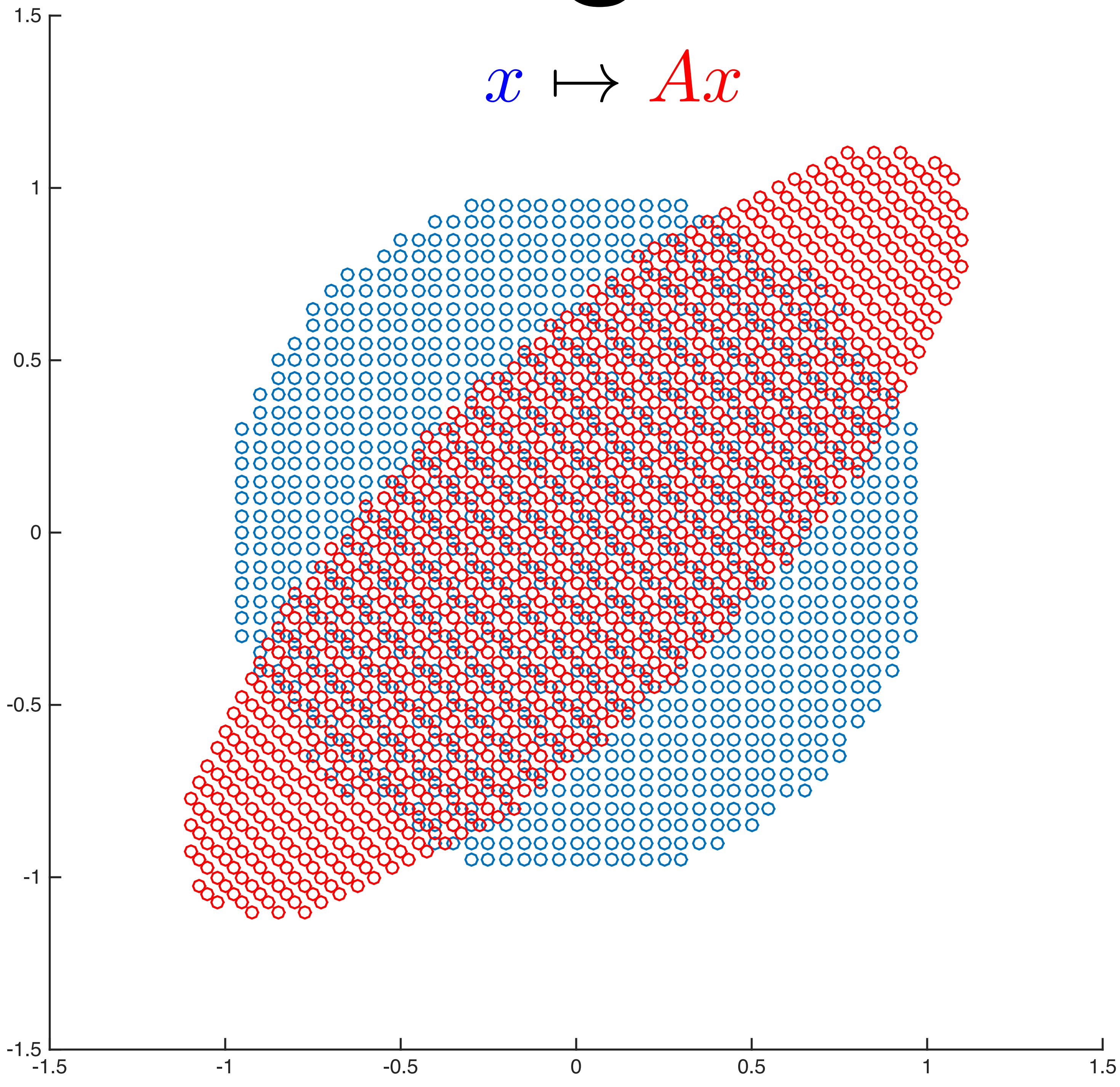

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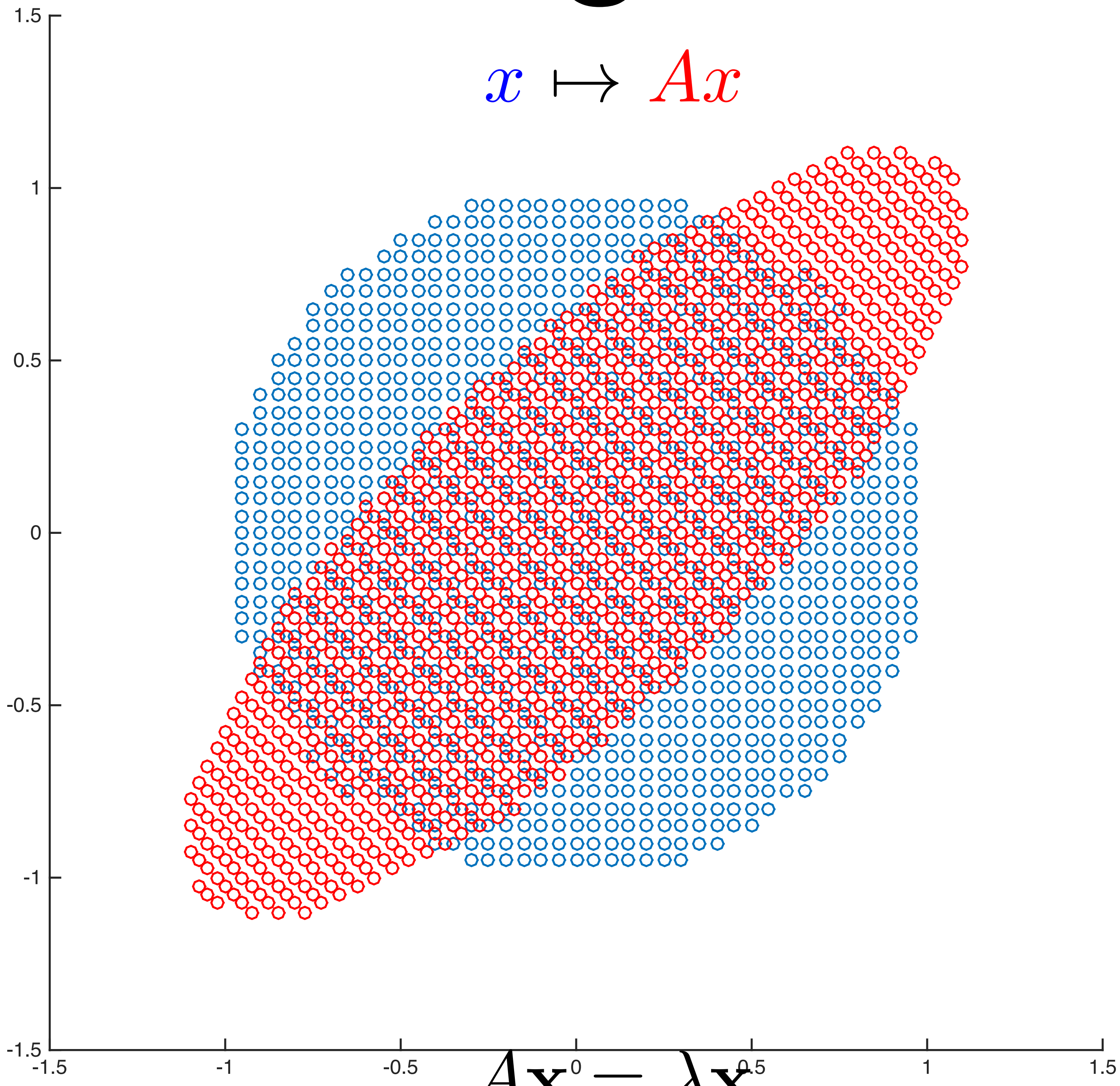

$$A\mathbf{x} = \lambda\mathbf{x}$$

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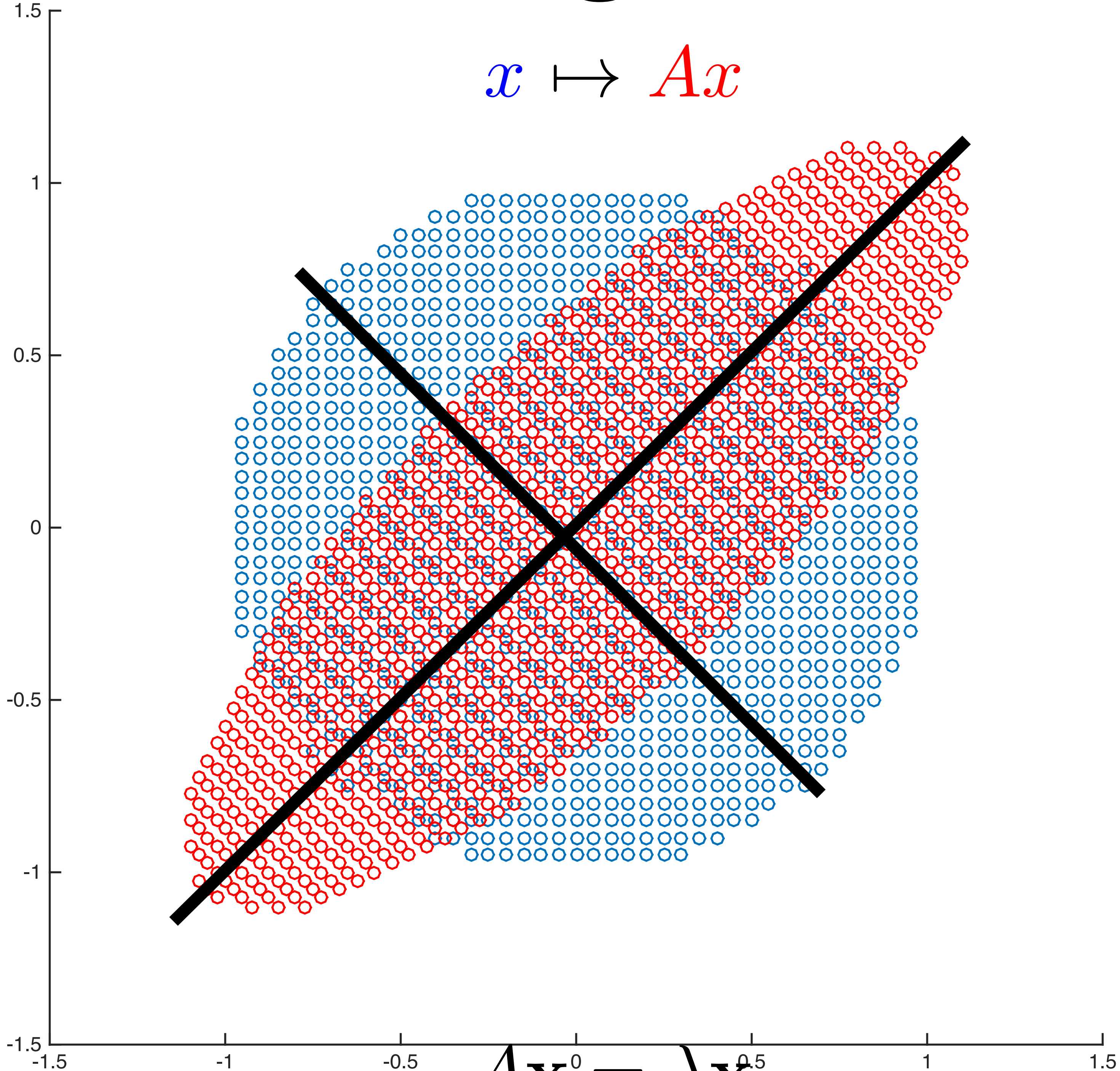

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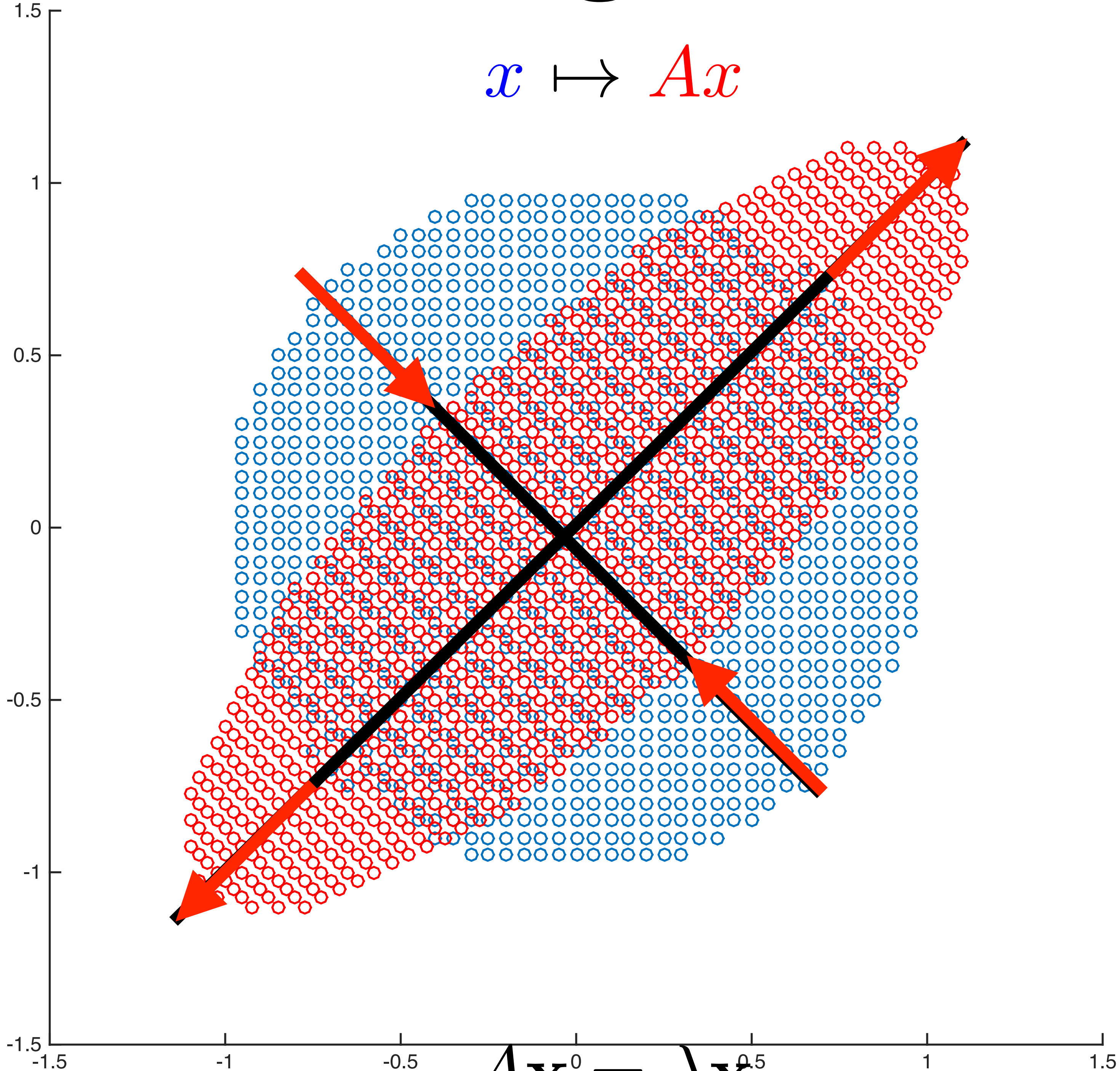

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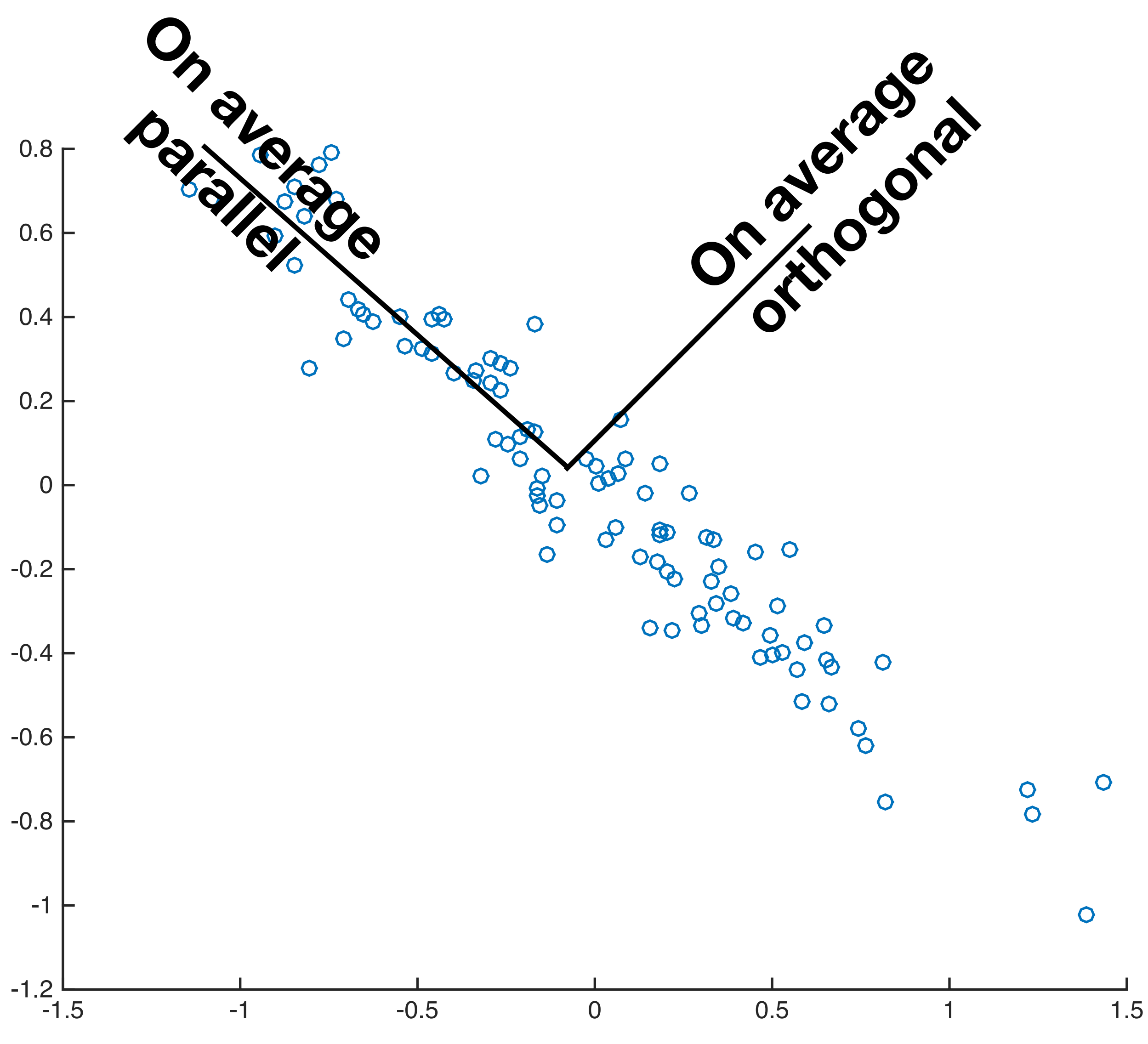

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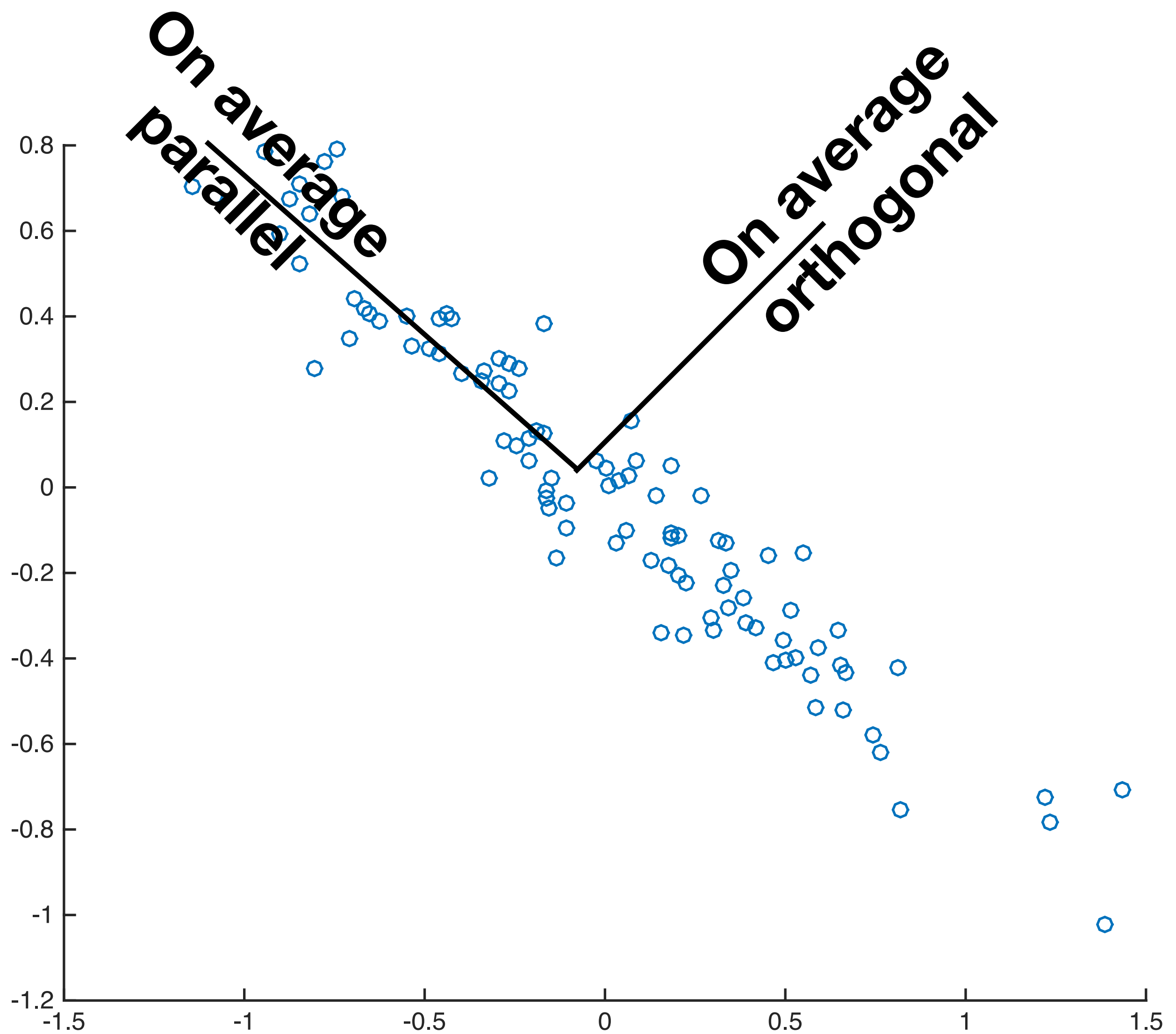

Top Eigenvector of covariance matrix

- 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?

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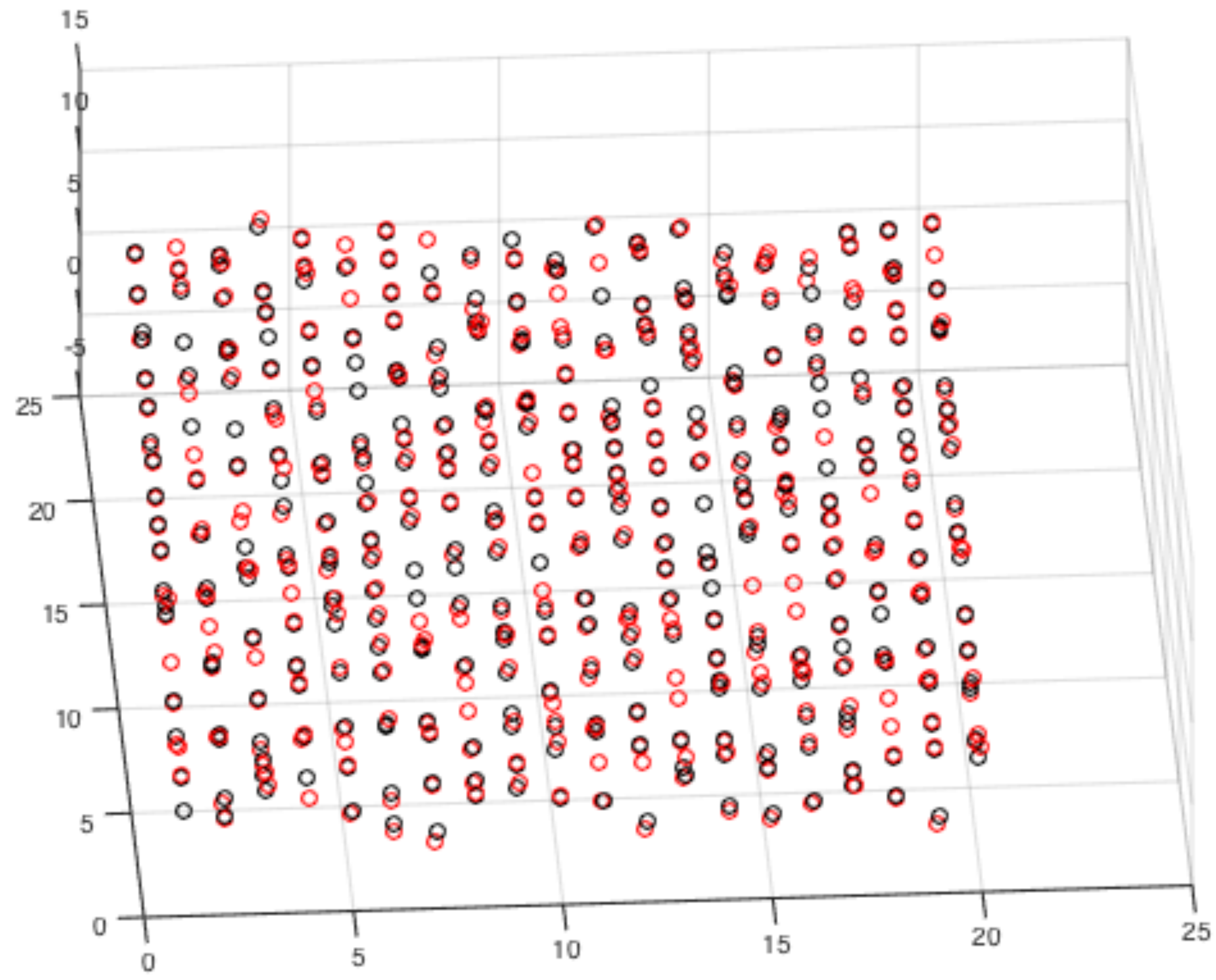
Ans: Maximize sum of spread in the K directions



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

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

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

Principal Component Analysis

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

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

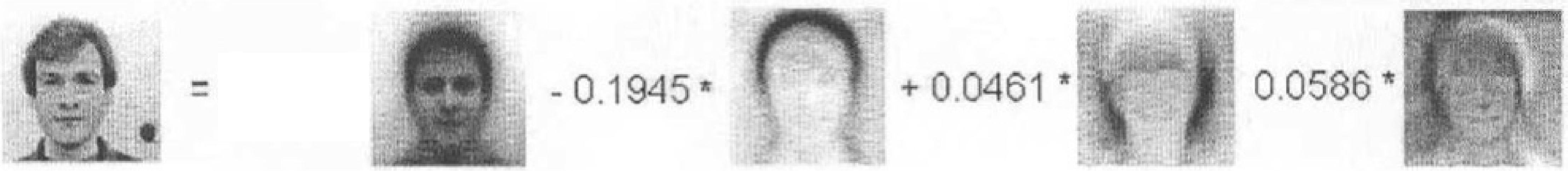
3. $Y = X \times W$

Demo

Principal Component Analysis (PCA)

Turk & Pentland'91

Eigen Face:



PRINCIPAL COMPONENT ANALYSIS (PCA)

Turk & Pentland'91

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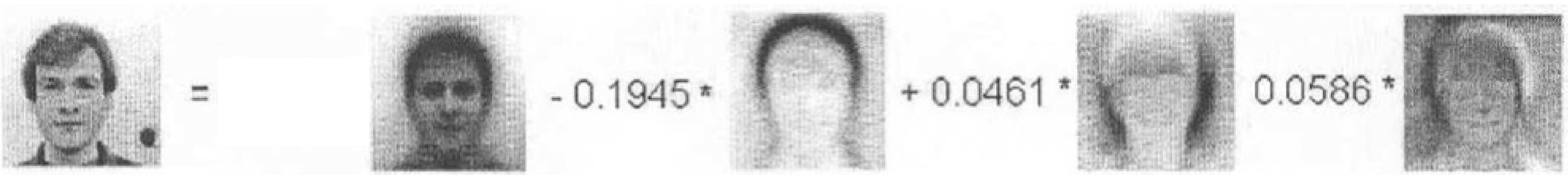

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Principal Component Analysis (PCA)

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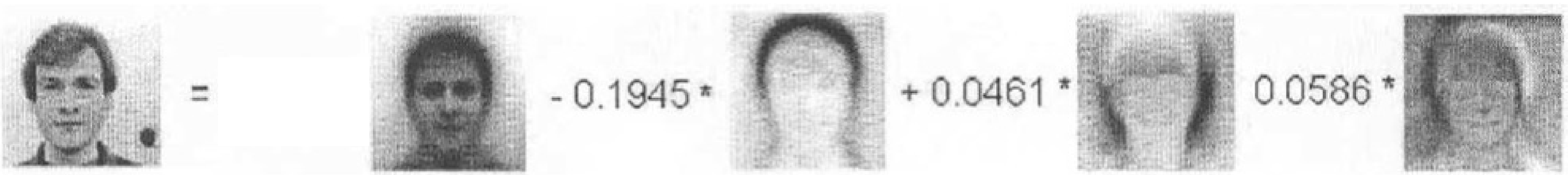

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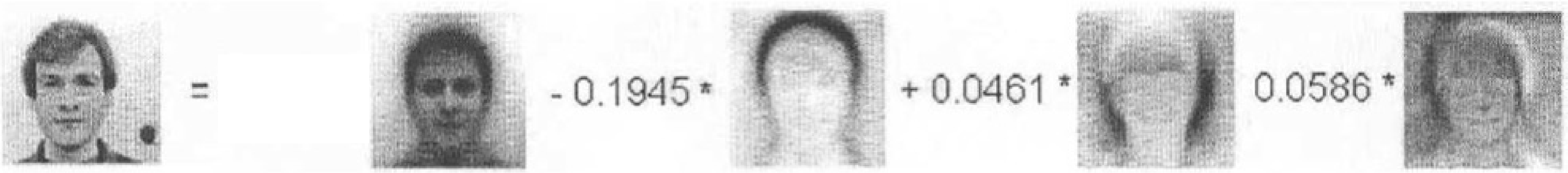

- Each x_t (each row of X) is a face image (vectorized version)
- Each y_t is the set of coefficients we multiply to the eigen face
- Each column of W is an Eigenface

Orthonormal Projections

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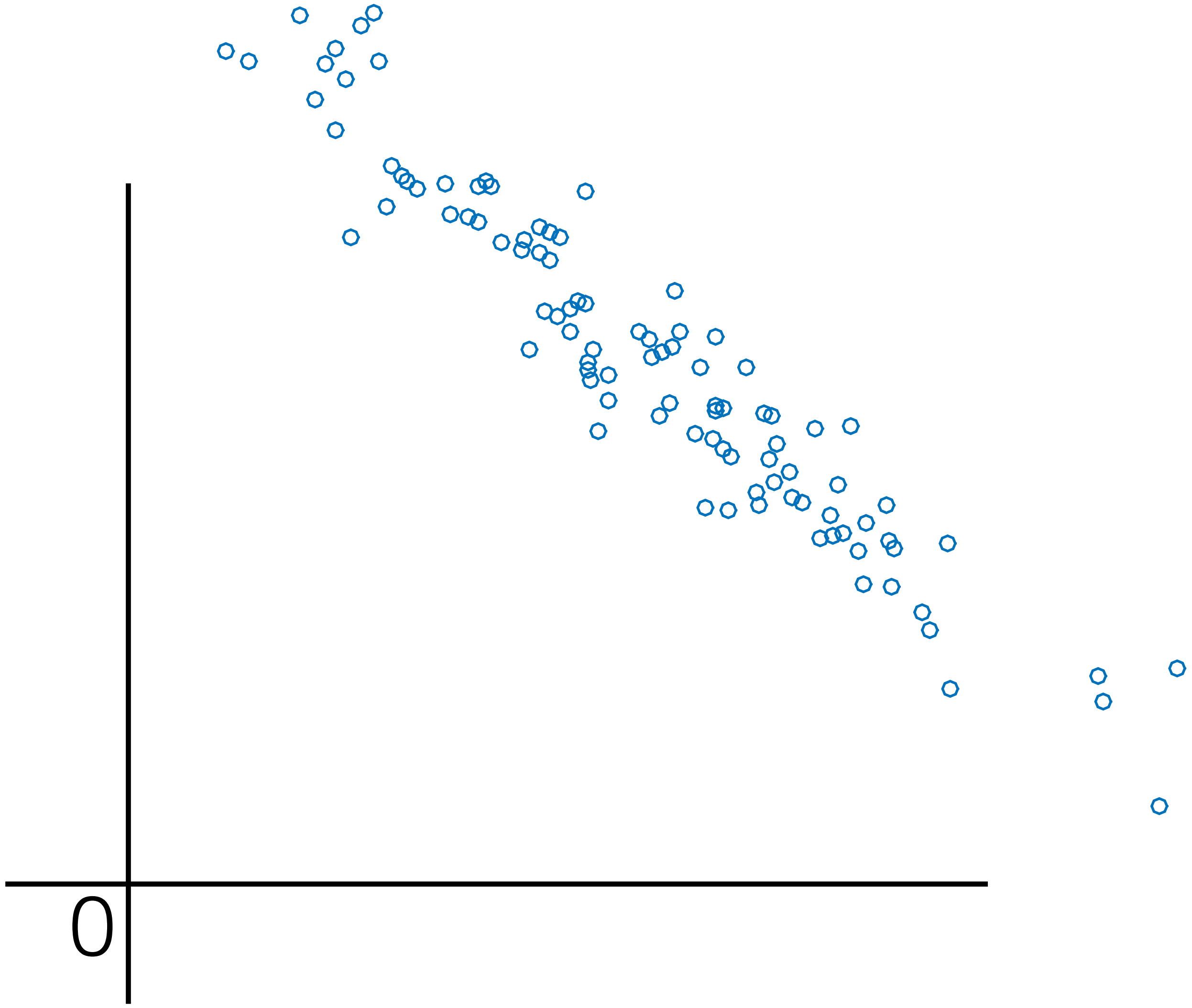
$$\|\mathbf{w}_i\|_2^2 = \sum_{k=1}^{d} \mathbf{w}_i[k]^2$$

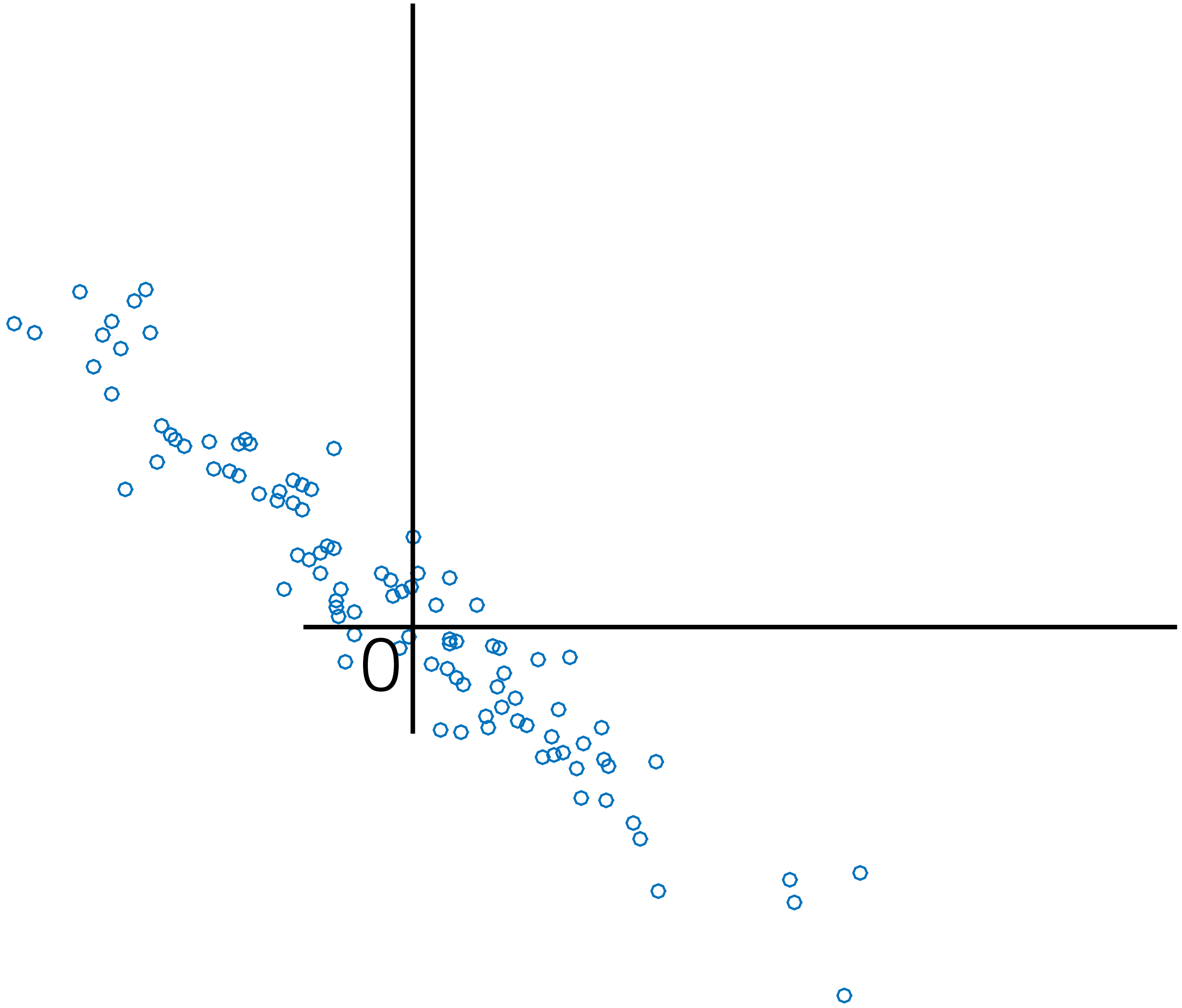
$$\mathbf{w}_i \perp \mathbf{w}_j \Rightarrow \sum_{k=1}^{d} \mathbf{w}_i[k]\mathbf{w}_j[k] = 0$$

CENTERING DATA



Compressing these data points…

Centering Data



… is same as compressing these.

Orthonormal Projections

- (Centered) Data-points as linear combination of some orthonormal basis, i.e.

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

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,

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

PCA: Minimizing Reconstruction Error

- Goal: find the basis that minimizes reconstruction error,

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&= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \sum_{j=1}^{d} \mathbf{y}_t[j]\mathbf{w}_j - \mu \right\|_2^2
\end{aligned}
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&= \left\| \sum_{j=K+1}^{d} \mathbf{y}_t[j]\mathbf{w}_j \right\|_2^2
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&= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \sum_{j=1}^{d} \mathbf{y}_t[j]\mathbf{w}_j - \mu \right\|_2^2 \\
&= \left\| \sum_{j=K+1}^{d} \mathbf{y}_t[j]\mathbf{w}_j \right\|_2^2 \quad (\text{but } \|a+b\|_2^2 = \|a\|_2^2 + \|b\|_2^2 + 2a^\top b)
\end{aligned}
$$

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\begin{aligned}
\|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 &= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \mathbf{x}_t \right\|_2^2 \\
&= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \sum_{j=1}^{d} \mathbf{y}_t[j]\mathbf{w}_j - \mu \right\|_2^2 \\
&= \left\| \sum_{j=K+1}^{d} \mathbf{y}_t[j]\mathbf{w}_j \right\|_2^2 \quad (\text{but } \|a+b\|_2^2 = \|a\|_2^2 + \|b\|_2^2 + 2a^\top b) \\
&= \left(\sum_{j=K+1}^{d} \mathbf{y}_t[j]^2 \|\mathbf{w}_j\|_2^2 + 2 \sum_{j=K+1}^{d} \sum_{i=j+1}^{d} \mathbf{y}_t[j]\mathbf{y}_t[i]\mathbf{w}_j^\top \mathbf{w}_i \right)
\end{aligned}
$$

PCA: Minimizing Reconstruction Error

- Goal: find the basis that minimizes reconstruction error,

$$
\begin{aligned}
\|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 &= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \mathbf{x}_t \right\|_2^2 \\
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&= \sum_{j=k+1}^{d} \mathbf{y}_t[j]^2 \|\mathbf{w}_j\|_2^2
\end{aligned}
$$

PCA: Minimizing Reconstruction Error

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&= \left\| \sum_{j=1}^{K} \mathbf{y}_t[j]\mathbf{w}_j + \mu - \sum_{j=1}^{d} \mathbf{y}_t[j]\mathbf{w}_j - \mu \right\|_2^2 \\
&= \left\| \sum_{j=K+1}^{d} \mathbf{y}_t[j]\mathbf{w}_j \right\|_2^2 \quad (\text{but } \|a+b\|_2^2 = \|a\|_2^2 + \|b\|_2^2 + 2a^\top b) \\
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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)
\end{aligned}$$

PCA: Minimizing Reconstruction Error

$$\frac{1}{n}\sum_{t=1}^{n}\|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 = \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2\|\mathbf{w}_j\|_2^2 \qquad (\text{but } \|\mathbf{w}_j\| = 1)$$

PCA: Minimizing Reconstruction Error

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$$= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2$$

PCA: Minimizing Reconstruction Error

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$$= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2 \quad (\text{now } \mathbf{y}_j = \mathbf{w}_j^\top(\mathbf{x}_t - \mu))$$

$$= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}(\mathbf{w}_j^\top(\mathbf{x}_t - \mu))^2$$

PCA: Minimizing Reconstruction Error

$$\frac{1}{n}\sum_{t=1}^{n}\|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 = \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2\|\mathbf{w}_j\|_2^2 \quad (\text{but } \|\mathbf{w}_j\| = 1)$$

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$$= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\left(\mathbf{w}_j^\top(\mathbf{x}_t - \mu)\right)^2$$

$$= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{w}_j^\top(\mathbf{x}_t - \mu)(\mathbf{x}_t - \mu)^\top\mathbf{w}_j$$

PCA: Minimizing Reconstruction Error

$$
\begin{aligned}
\frac{1}{n}\sum_{t=1}^{n}\|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 &= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2\|\mathbf{w}_j\|_2^2 \quad (\text{but } \|\mathbf{w}_j\| = 1) \\
&= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{y}_t[j]^2 \quad (\text{now } \mathbf{y}_j = \mathbf{w}_j^\top(\mathbf{x}_t - \mu)) \\
&= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}(\mathbf{w}_j^\top(\mathbf{x}_t - \mu))^2 \\
&= \frac{1}{n}\sum_{t=1}^{n}\sum_{j=k+1}^{d}\mathbf{w}_j^\top(\mathbf{x}_t - \mu)(\mathbf{x}_t - \mu)^\top\mathbf{w}_j \\
&= \sum_{j=k+1}^{d}\mathbf{w}_j^\top\Sigma\mathbf{w}_j
\end{aligned}
$$

PCA: Minimizing Reconstruction Error

$$\text{Claim: } \sum_{j=1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j = \text{ Constant } = \frac{1}{n}\sum_{t=1}^{n} \|x_t - \mu\|_2^2$$

PCA: Minimizing Reconstruction Error

Claim: $\sum_{j=1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j = \text{ Constant } = \frac{1}{n}\sum_{t=1}^{n} \|x_t - \mu\|_2^2$

Recall that: $\frac{1}{n}\sum_{t=1}^{n} \|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 = \sum_{j=K+1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j$

PCA: Minimizing Reconstruction Error

Claim: $\sum_{j=1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j = \text{ Constant } = \frac{1}{n}\sum_{t=1}^{n} \|x_t - \mu\|_2^2$

Recall that: $\frac{1}{n}\sum_{t=1}^{n} \|\hat{\mathbf{x}}_t - \mathbf{x}_t\|_2^2 = \sum_{j=K+1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j$

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

PCA: Minimizing Reconstruction Error

Minimize w.r.t. $\mathbf{w}_1, \ldots, \mathbf{w}_K$'s that are orthonormal,

$$\underset{\forall j,\ \|\mathbf{w}_j\|_2 = 1}{\operatorname{argmin}} \sum_{j=k+1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j$$

PCA: Minimizing Reconstruction Error

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&\underset{\forall j,\ \|\mathbf{w}_j\|_2=1}{\operatorname{argmin}} \sum_{j=k+1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j \\
&= \underset{\forall j,\ \|\mathbf{w}_j\|_2=1}{\operatorname{argmin}} \left(\frac{1}{n} \sum_{t=1}^{n} \|\hat{\mathbf{x}}_t - \mu\|_2^2 - \sum_{j=1}^{K} \mathbf{w}_j^\top \Sigma \mathbf{w}_j \right)
\end{aligned}$$

PCA: Minimizing Reconstruction Error

Minimize w.r.t. $\mathbf{w}_1, \ldots, \mathbf{w}_K$'s that are orthonormal,

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&\underset{\forall j,\ \|\mathbf{w}_j\|_2=1}{\operatorname{argmin}} \sum_{j=k+1}^{d} \mathbf{w}_j^\top \Sigma \mathbf{w}_j \\
&= \underset{\forall j,\ \|\mathbf{w}_j\|_2=1}{\operatorname{argmin}} \left(\frac{1}{n} \sum_{t=1}^{n} \|\hat{\mathbf{x}}_t - \mu\|_2^2 - \sum_{j=1}^{K} \mathbf{w}_j^\top \Sigma \mathbf{w}_j \right) \\
&= \underset{\|\mathbf{w}_j\|_2=1, \mathbf{w}_j \perp \mathbf{w}_k}{\operatorname{argmax}} \sum_{j=1}^{K} \mathbf{w}_j^\top \Sigma \mathbf{w}_j
\end{aligned}$$

Maximize Total Spread = Minimize Reconstruction Error

Principal Component Analysis

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

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

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

Reconstruction

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

Principal Component Analysis: Demo