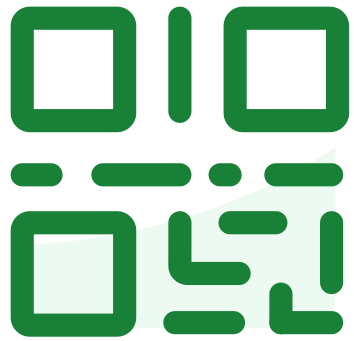


Do not edit
How to change the
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Lecture 3

Dimensionality Reduction

PCA with a review of linear algebra, calculus, and optimization

EECS 189/289, Fall 2026 @ UC Berkeley

Joseph E. Gonzalez and Narges Norouzi

Recap



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In Tuesday's lecture we focused on **Nearest Neighbor** methods:

- **Non-parametric Classification and Regression** – use the labels of the k -nearest neighbors to estimate the test point.
- **K-means clustering** – grouping nearby points.

Today we will explore **Principal Component Analysis (PCA)**

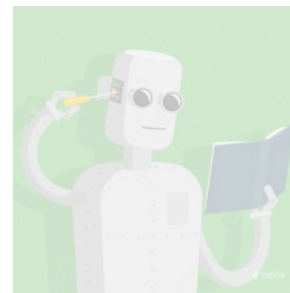
- **Dimensionality reduction** – we will project high-dimensional data into a descriptive low-dimensional space.
- **Parametric method** – there will be a fixed set of parameters

We will review **linear algebra, calculus, and optimization.**

Taxonomy of Machine Learning



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Labeled Data

Reward

Unlabeled Data

Supervised Learning

Reinforcement Learning

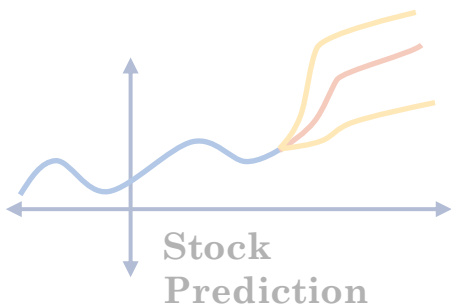
Unsupervised Learning

Quantitative Label

Categorical Label

Regression

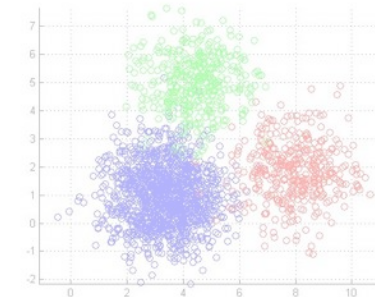
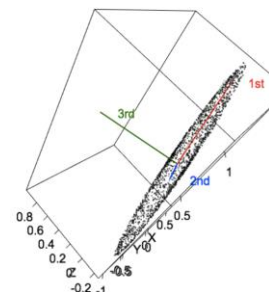
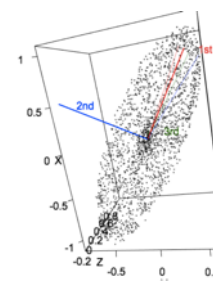
Classification



Alpha Go

Dimensionality Reduction

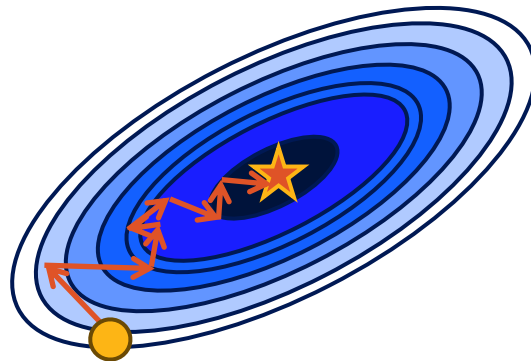
Clustering



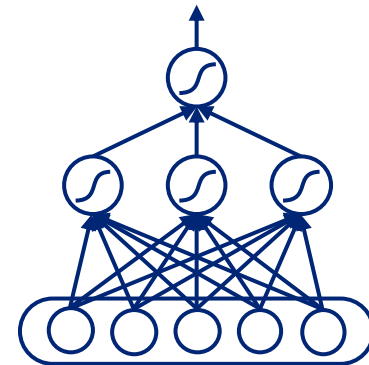
Using PCA and scikit-learn to make sense of congressional votes.

Demo

Algorithm



Model



Application



This Machine Learning Class

Interpreting the demonstration



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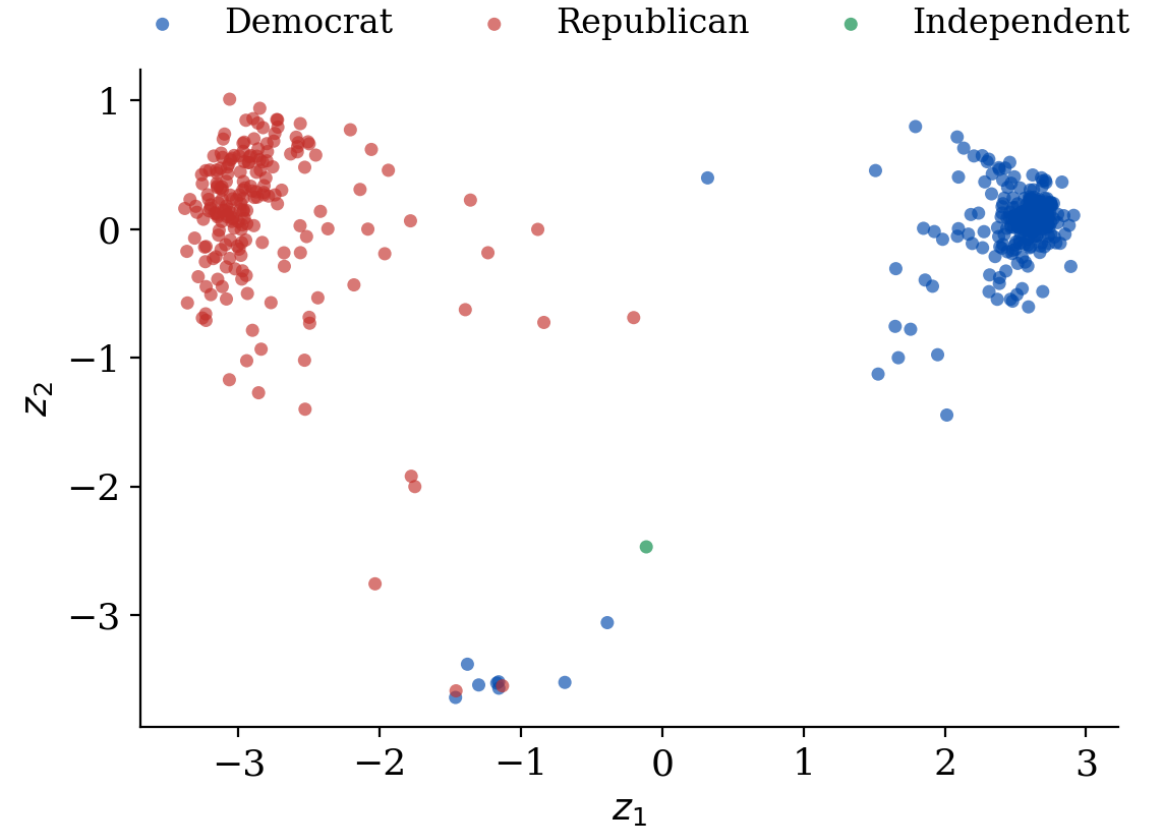
Input Data ($\mathbb{R}^{441 \times 41}$): 441 legislators and 41 roll calls all 0/1s

Transformed Data ($\mathbb{R}^{441 \times 2}$): reduced to 441 points into two dimensions.

- The choice of 2 dimensions was a hyper-parameter decision.

Interesting Observations

- The sign of the first coordinate agrees with party affiliation for **98%** of the House
- **No party label** was supplied to the algorithm. The input consisted of **just votes**.
- The fitted **model** consists of **two vectors** of **41 numbers**. (the parameters)



How does PCA construct this low-dimensional representation of the data?

Objective of Dimensionality Reduction



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High-dimensional data (many columns) and can be difficult to **visualize** and **model**.

- Challenging to **plot** more than a few dimensions
- Some **modeling** techniques perform poorly **in high-dimensions** (e.g., k-NN and k-Means)

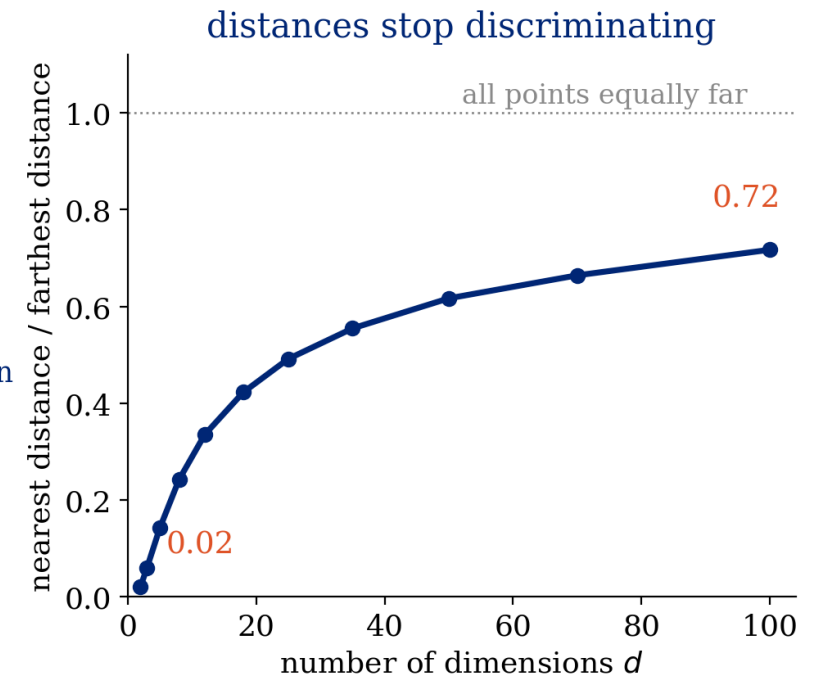
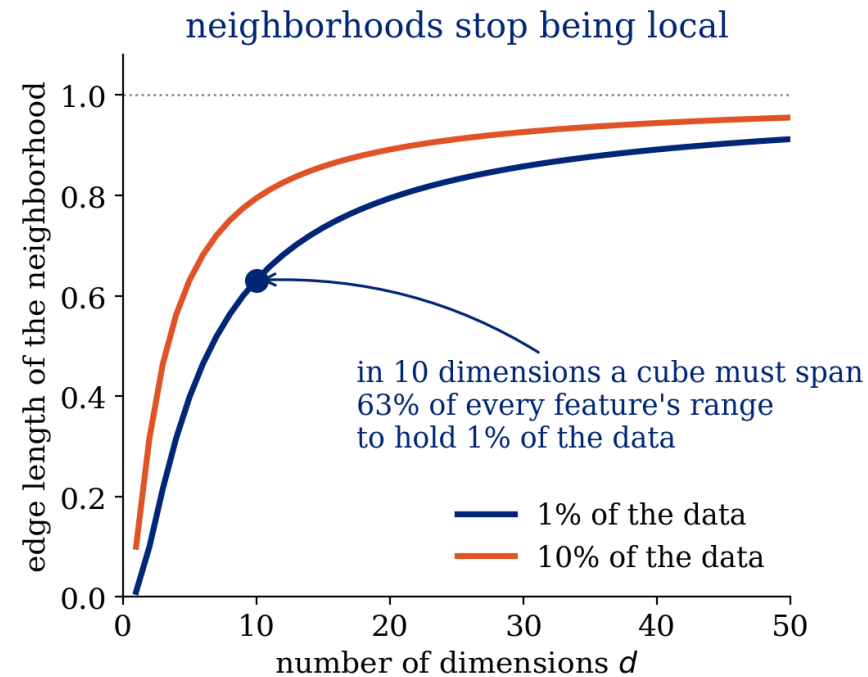
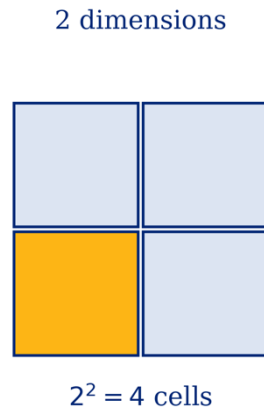
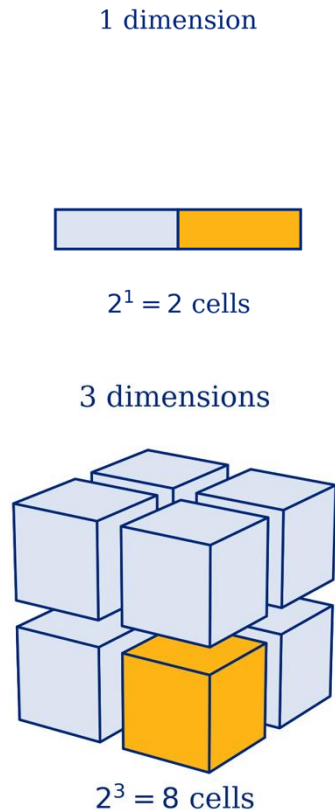
The Curse of Dimensionality



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Volume grows exponentially with d :

- **Neighborhoods stop being local:** a box holding 1% of the data spans most of every axis
- **Distances stop discriminating:** the nearest and farthest points become almost equally far



441 legislators in 41 dimensions: splitting each axis once gives $2^{41} \approx 2$ trillion cells for 441 points.



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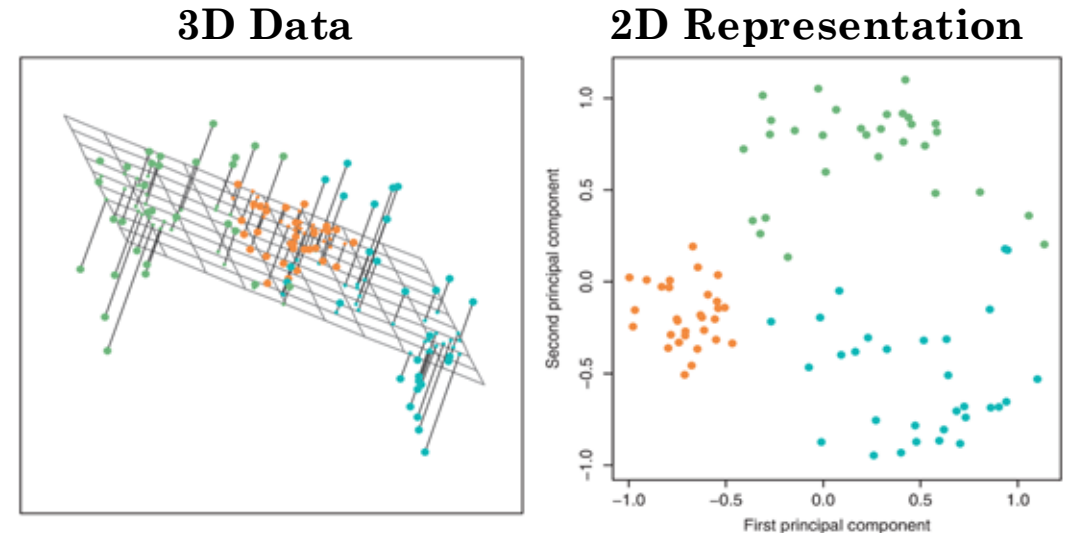
Objective of Dimensionality Reduction

High-dimensional data (many columns) and can be difficult to **visualize** and **model**.

- Challenging to **plot** more than a few dimensions
- Some **modeling** techniques perform poorly **in high-dimensions** (e.g., k-NN and k-Means)

Often high-dimensional data **can be compressed** into a **lower dimensional space** with minimal loss of information.

Dimensionality reduction: take high-dimensional data and map it to a lower dimensional space that **preserves as much information** as possible.



Formulating the Problem



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The Rank of a Matrix

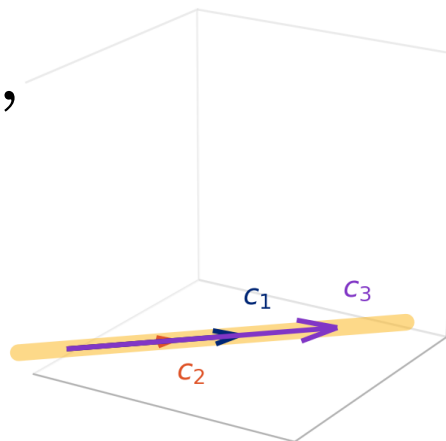
The **rank** of a matrix is:

- the dimension of the **space spanned by the columns**.
- the **maximum number of *linearly independent* columns**.

A **column** is **linearly independent** of all other columns if it cannot be expressed as a linear combination of the other columns.

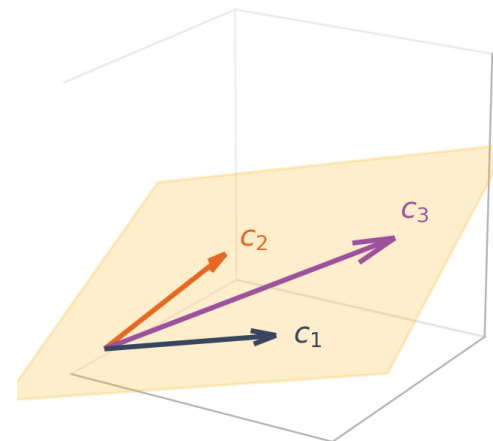
The **rank(X) $\leq \min(n, d)$** ,
and a matrix that attains
this bound is said to
have **full rank**.

rank 1



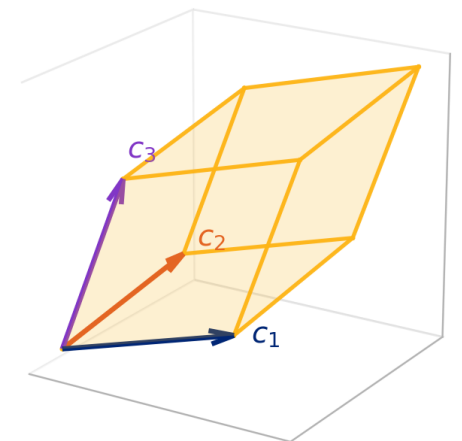
the span is a line
every column is a multiple of one direction

rank 2



the span is a plane
 $c_3 = c_1 + c_2$, adding nothing new

rank 3



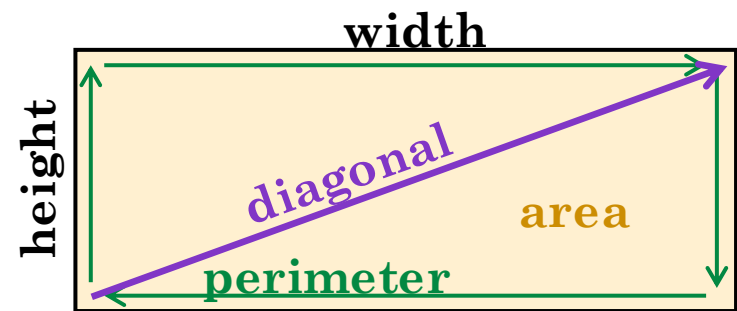
the span is all of $\mathbb{R}^3$
no column is a combination of the others



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Simple Example

Suppose I have a large table of random rectangles along with **properties** of those rectangles:



width	height	perimeter	area	diagonal
7	6	26	42	9.22
4	6	20	24	7.21
5	2	14	10	5.39
7	4	22	28	8.06
3	5	16	15	5.83

What is the **rank** of this dataset?

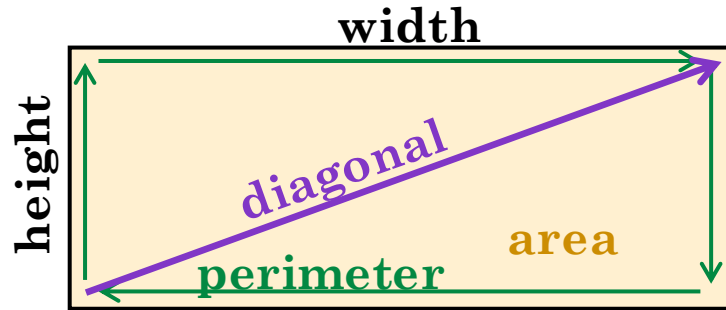


What is the rank of the following dataset?

Rank of the Rectangles Example



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width	height	perimeter	area	diagonal
7	6	26	42	9.22
4	6	20	24	7.21
5	2	14	10	5.39
7	4	22	28	8.06
3	5	16	15	5.83

5 columns, rank 4

the perimeter column is redundant, so
the matrix is not full rank

$$\text{perimeter} = 2w + 2h$$

*a linear combination of the
other two columns*

$$\text{area} = w \times h$$

not a linear combination

$$\text{diagonal} = \sqrt{w^2 + h^2}$$

not a linear combination

How many dimensions (columns) are really needed?



How many dimensions are needed to fully describe this dataset?

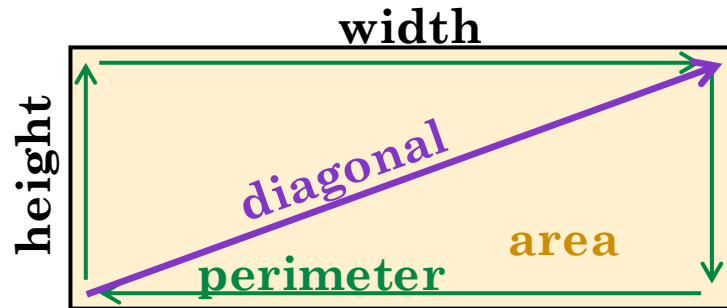


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Intrinsic Dimension and Matrix Rank

The **intrinsic dimension** is the minimum number of variables needed to describe the data.

- Unlike rank, intrinsic dimension allows **nonlinear relationships between variables**.



$$\text{perimeter} = 2w + 2h$$

a linear combination of the other two columns

$$\text{area} = w \times h$$

not a linear combination

$$\text{diagonal} = \sqrt{w^2 + h^2}$$

not a linear combination

5 columns, rank 4

the perimeter column is redundant, so the matrix is not full rank

Intrinsic Dimension is 2

every column is determined by w and h alone

Every column of that table is determined by the **width** w and the **height** h .



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Real data is rarely *exactly* low rank

Measure the perimeter with a tape measure instead of computing it, and the exact relationship is destroyed → **the rank returns to 5.**

- Small amounts of **noise** can make data full rank.

Example: the congressional vote matrix from the demo

Full Rank (41)

nothing may be discarded

Rank 2 Approx. → 86%

of the spread in the data

Typically, datasets are nearly **full rank** but are often accurately approximated by a **lower dimensional sub-space** (close to the **intrinsic dimension**).

How do we find a lower dimensional representation that accurately approximates the data?

Deriving PCA

The input Data Matrix



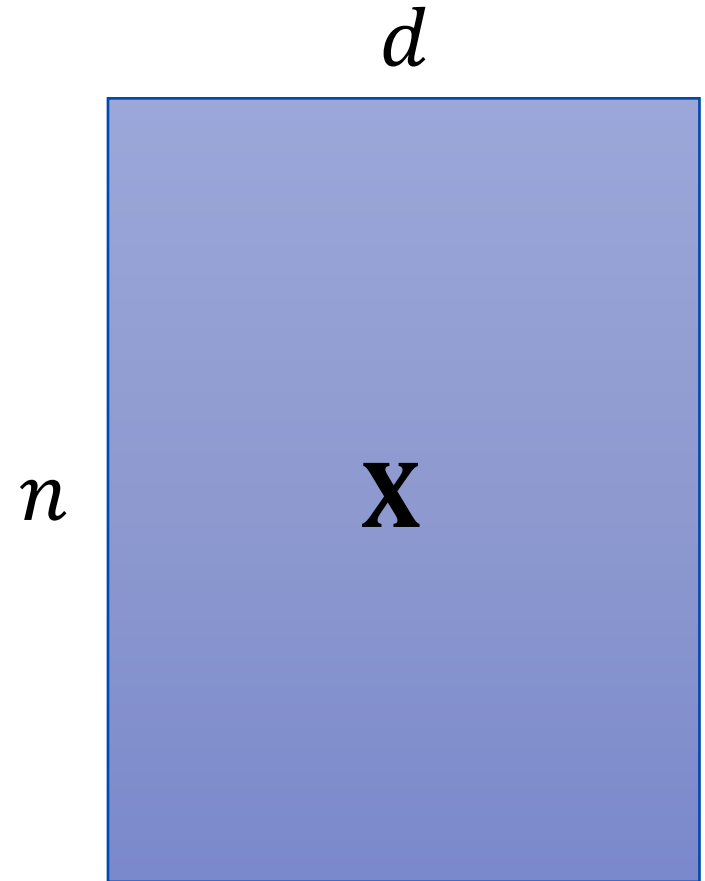
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For n datapoints and d features:

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

The i -th row is a **single datapoint**, written as
a **row vector** with d entries:

$$\mathbf{X}_i \in \mathbb{R}^{1 \times d}$$



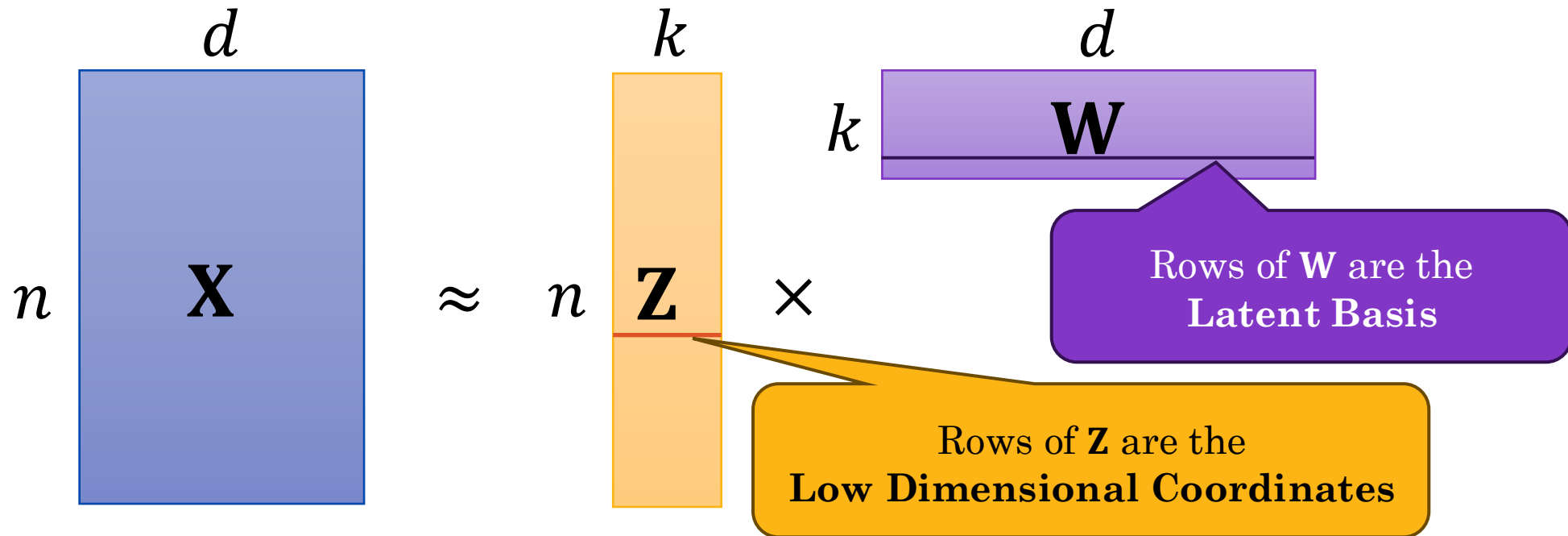
Dimensionality reduction as Matrix Factorization



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Goal: Construct a matrix $\mathbf{Z} \in \mathbb{R}^{n \times k}$ of size $n \times k$ and a matrix $\mathbf{W} \in \mathbb{R}^{k \times d}$ of size $k \times d$ whose product reproduces $\mathbf{X}$ as closely as possible:

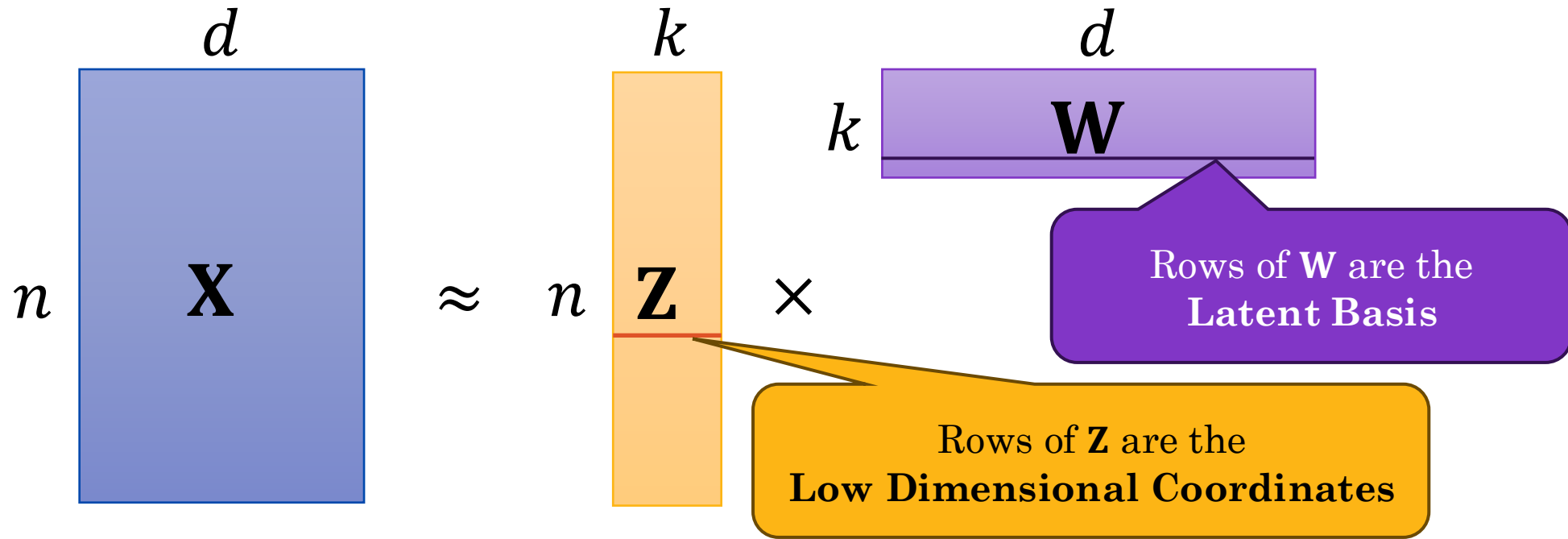
$$\mathbf{X} \approx \mathbf{Z}\mathbf{W}$$



Interpretation of Z and W



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Each **row of W** determines the basis of the **subspace of X** used to approximate the data. (*These will become our Principal Components give the opt. problem.*)

Each **row of Z** determines the “mix” of the rows of W used to reconstruct a row in the original data.

Which of these products can equal $\mathbf{X}$ exactly?



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Suppose $\mathbf{X} \in \mathbb{R}^{3 \times 3}$ is a any 3×3 matrix with full rank. Which factorizations could always exactly reconstruct $\mathbf{X}$.

- A. $(3 \times 2) \times (2 \times 3)$
- B. $(3 \times 3) \times (3 \times 3)$
- C. $(3 \times 1) \times (1 \times 3)$
- D. $(3 \times 4) \times (4 \times 3)$
- E. Something else





Suppose $\mathbf{X} \in \mathbb{R}^{(3 \times 3)}$ is a any 3×3 matrix with full rank. Which factorizations could always exactly reconstruct $\mathbf{X}$.



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The rank of the product is bounded by k

Suppose $\mathbf{X} \in \mathbb{R}^{3 \times 3}$ is a any 3×3 matrix with full rank. Which factorizations could always exactly reconstruct $\mathbf{X}$.

- A. $(3 \times 2) \times (2 \times 3)$
 - B. $(3 \times 3) \times (3 \times 3)$
 - C. $(3 \times 1) \times (1 \times 3)$
 - D. $(3 \times 4) \times (4 \times 3)$
- $\text{rank}(\mathbf{ZW}) \leq \min(\text{rank } \mathbf{Z}, \text{rank } \mathbf{W}) \leq k$**
- **B** and **D** can reproduce $\mathbf{X}$ exactly, but achieve no reduction
 - **A** and **C** cannot (in general), since their inner dimension is smaller than the rank of $\mathbf{X}$

In practice k is chosen below the rank of $\mathbf{X}$, so that $\mathbf{ZW}$ is necessarily an approximation.

**Among all factorizations of rank k ,
which one is best?**



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Defining an objective function

The product $\mathbf{Z}_i \mathbf{W}$ is our reconstruction of the datapoint $\mathbf{X}_i$. We evaluate a choice of $(\mathbf{Z}, \mathbf{W})$ by the **average squared error** of that reconstruction:

$$\text{Loss}(\mathbf{Z}, \mathbf{W}) = \frac{1}{n} \sum_{i=1}^n \|\mathbf{X}_i - \mathbf{Z}_i \mathbf{W}\|^2$$

Squared
Euclidean Norm

$$\|\mathbf{a}\|^2 = \sum_{i=1}^d a_i^2$$

X is assumed to be centered

that is, the mean of each column has been subtracted.

This is an optimization problem

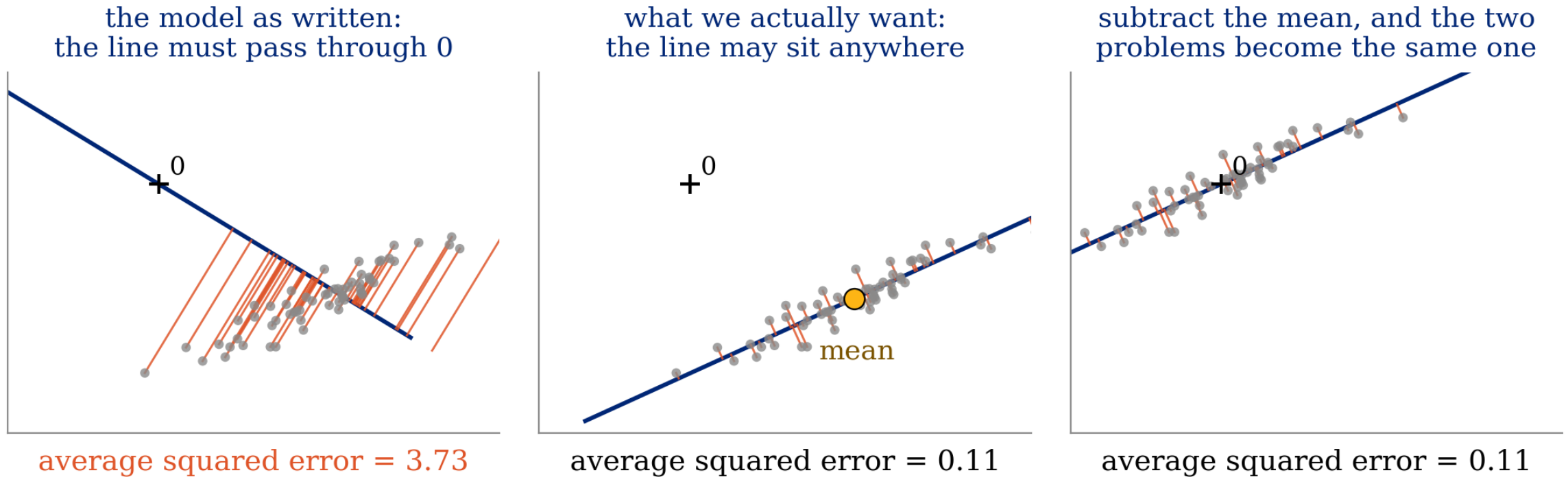
The parameters are $\mathbf{Z}$ and $\mathbf{W}$, and there is a single quantity to be minimized. **It is the first of many such problems this semester.**



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Why we subtract the mean

As written, the model $\mathbf{X} \approx \mathbf{Z}\mathbf{W}$ places every reconstruction on a subspace through the origin. The origin is an arbitrary point, and the data has no reason to lie near it.



**The best fitting subspace always passes through the mean,
so we subtract the mean first.**



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The Factorization is Not Unique

For any invertible $k \times k$ matrix $\mathbf{A}$:

$$\mathbf{Z}\mathbf{W} = (\mathbf{Z}\mathbf{A}^{-1})(\mathbf{A}\mathbf{W})$$

- The reconstruction is identical, while $\mathbf{Z}$ and $\mathbf{W}$ are entirely different.
- Alternatively, $\mathbf{W}$ may be scaled down and $\mathbf{Z}$ scaled up without affecting the objective.

We remove the scale ambiguity by requiring the rows of $\mathbf{W}$ to be orthonormal

$$\mathbf{W}\mathbf{W}^T = \mathbf{I}$$

- Row vectors of $\mathbf{W}$ are unit length: $\mathbf{w}_i\mathbf{w}_i^T = 1$
- Row vectors of $\mathbf{W}$ are orthogonal: $\mathbf{w}_i\mathbf{w}_j^T = 0$ for all $i \neq j$

Nothing is lost by doing so, since every k -dimensional subspace admits an **orthonormal basis**.



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The Full Optimization Problem

Determine the values of $(\mathbf{Z}, \mathbf{W})$ that **minimize** the **average squared error** of that reconstruction:

$$(\mathbf{Z}^*, \mathbf{W}^*) = \arg \min_{\mathbf{Z} \in \mathbb{R}^{n \times k}, \mathbf{W} \in \mathbb{R}^{k \times d}} \left(\frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{z}_i \mathbf{W}\|^2 \right)$$

subject to the **row orthonormality constraints**:

$$\mathbf{W} \mathbf{W}^\top = \mathbf{I}$$

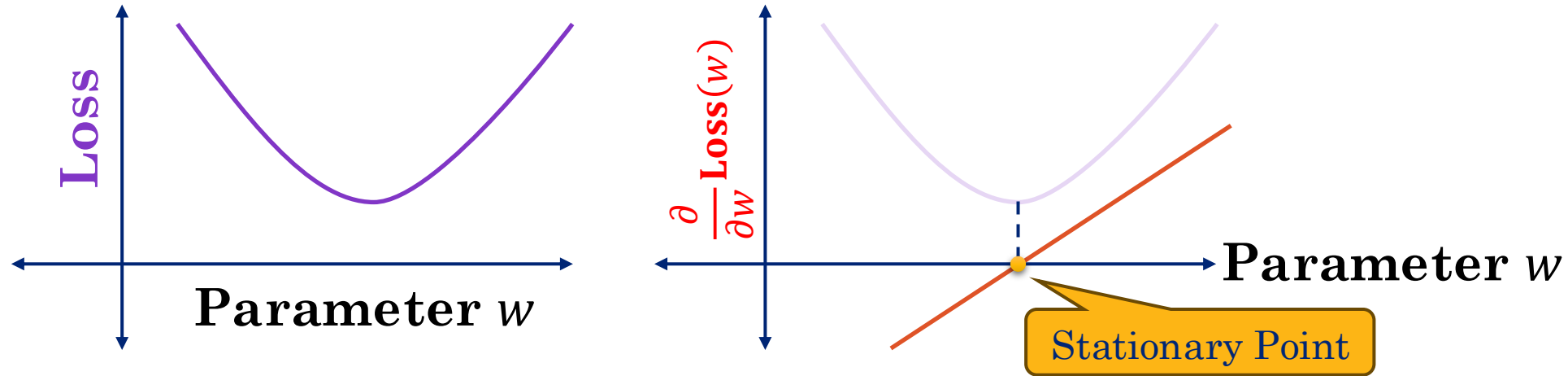
Plan:

1. Optimize $\mathbf{Z}$ in terms of $\mathbf{W}$ (**Stationary Point Method**)
2. Optimize $\mathbf{W}$ with constraints (**Method of Lagrange Multipliers**)



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The *Basic* Stationary Point Method



- **Differentiate** with respect to each parameter
- Set the **derivatives to zero and solve**
- **(Optional)** verify that second derivative is positive.

$$\frac{\partial}{\partial w} \text{Loss}(w) = 0$$

This procedure applies when the objective is **smooth** and the **resulting equations can be solved**. All conditions hold today, and we obtain an exact solution.

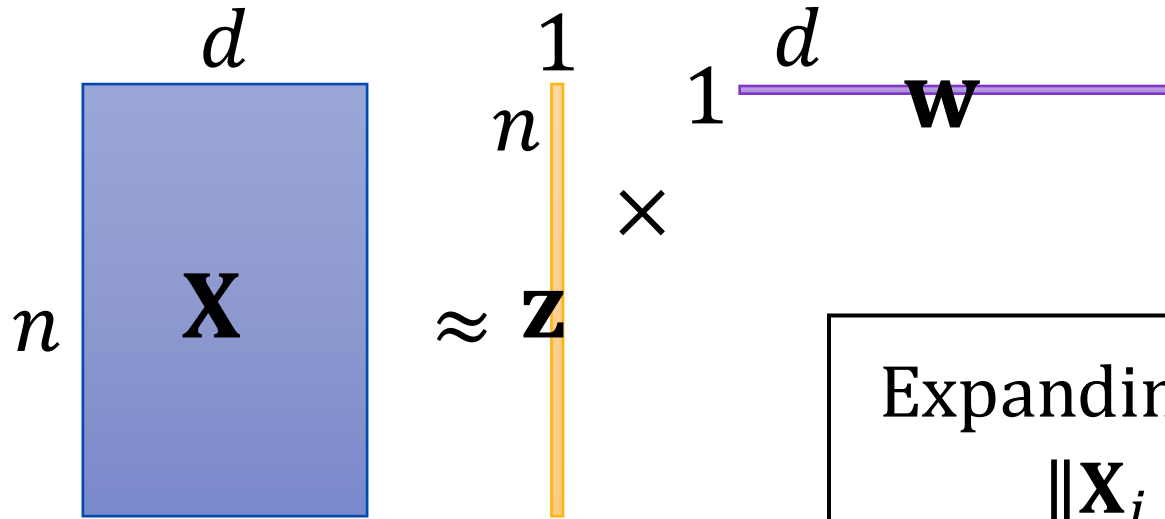


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Case $k = 1$ (Rank 1 Factorization)

A single unit direction $\mathbf{w} \in \mathbb{R}^{1 \times d}$, with $\mathbf{w}\mathbf{w}^\top = \mathbf{1}$

A single coefficient $z_i \in \mathbb{R}$ for each datapoint (row) in $\mathbf{X}$



$$\text{Loss}(\mathbf{z}, \mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \|\mathbf{X}_i - z_i \mathbf{w}\|^2$$

Expanding the Loss

$$\begin{aligned} \|\mathbf{X}_i - z_i \mathbf{w}\|^2 &= (\mathbf{X}_i - z_i \mathbf{w})(\mathbf{X}_i - z_i \mathbf{w})^\top \\ &= \underbrace{\mathbf{X}_i \mathbf{X}_i^\top}_{\text{Constant with respect to } (\mathbf{z}, \mathbf{w})} - 2z_i \mathbf{X}_i \mathbf{w}^\top + z_i^2 \underbrace{\mathbf{w} \mathbf{w}^\top}_{\substack{1 \\ \text{(orthonormality constraint)}}} \end{aligned}$$

Simplified Loss

$$\text{Loss}(\mathbf{z}, \mathbf{w}) = C + \frac{1}{n} \sum_{i=1}^n (-2z_i \mathbf{X}_i \mathbf{w}^\top + z_i^2)$$

Computing the Stationary Point z_i^*

$$\text{Loss}(\mathbf{z}, \mathbf{w}) = C + \frac{1}{n} \sum_{i=1}^n (-2z_i \mathbf{X}_i \mathbf{w}^\top + z_i^2)$$



Take the **derivative of the loss** with **respect to the parameter** (z_i) that we want to optimize

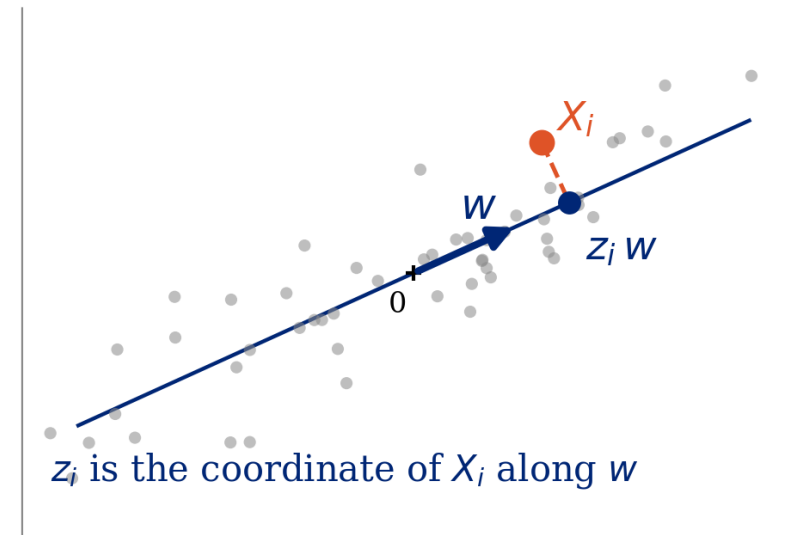
$$\frac{\partial}{\partial z_i} \text{Loss}(\mathbf{z}, \mathbf{w}) = -2 \frac{1}{n} \mathbf{X}_i \mathbf{w}^\top + 2 \frac{1}{n} z_i$$

Set the derivative equal to zero and solve for the parameter

$$-2 \frac{1}{n} \mathbf{X}_i \mathbf{w}^\top + 2 \frac{1}{n} z_i = 0 \quad \Rightarrow \quad z_i = \mathbf{X}_i \mathbf{w}^\top$$

The optimal value for z_i is **the projection**:

$$z_i^* = \mathbf{X}_i \mathbf{w}^\top$$



Substituting the solution for $\mathbf{z}^*$

$$\text{Loss}(\mathbf{z}, \mathbf{w}) = C + \frac{1}{n} \sum_{i=1}^n (-2z_i \mathbf{X}_i \mathbf{w}^\top + z_i^2)$$



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We derived z_i^* in terms of $\mathbf{w}$ so we can rewrite the loss in terms of only $\mathbf{w}$:

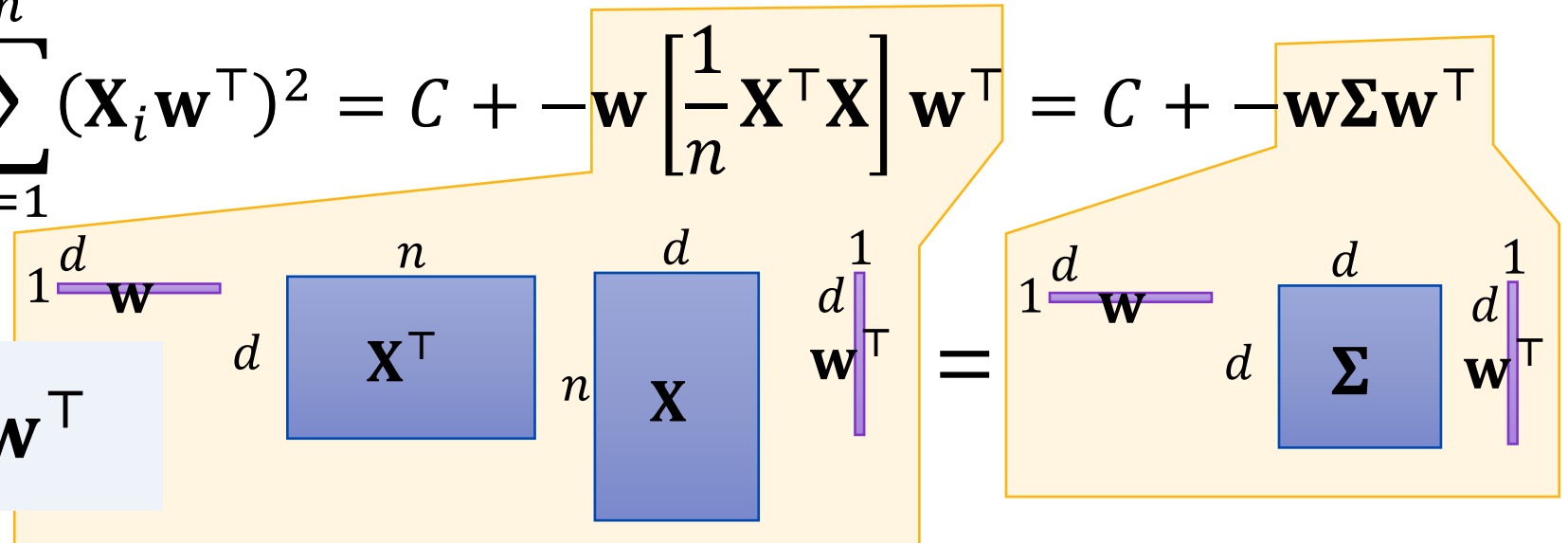
$$z_i^* = \mathbf{X}_i \mathbf{w}^\top$$

$$\text{Loss}(\mathbf{w}) = C + \frac{1}{n} \sum_{i=1}^n (-2(\mathbf{X}_i \mathbf{w}^\top) \mathbf{X}_i \mathbf{w}^\top + (\mathbf{X}_i \mathbf{w}^\top)^2)$$

Simplifying terms:

$$\text{Loss}(\mathbf{w}) = C + -\frac{1}{n} \sum_{i=1}^n (\mathbf{X}_i \mathbf{w}^\top)^2 = C + -\mathbf{w} \left[\frac{1}{n} \mathbf{X}^\top \mathbf{X} \right] \mathbf{w}^\top = C + -\mathbf{w} \Sigma \mathbf{w}^\top$$

$$\text{Loss}(\mathbf{w}) = C - \mathbf{w} \Sigma \mathbf{w}^\top$$





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Constrained Optimization for $\mathbf{w}$

We want to minimize the loss with respect to $\mathbf{w}$ (what could go wrong?)

$$\text{Loss}(\mathbf{w}) = \mathbf{C} - \mathbf{w}\Sigma\mathbf{w}^\top$$

If you naively optimize this loss with respect to $\mathbf{w}$ you can make it arbitrarily negative by making $\mathbf{w}$ **arbitrarily large**.

We still need to account for the **row orthonormality constraint**:

$$\mathbf{w}\mathbf{w}^\top = \mathbf{I}$$

The constraint is essential: it is what makes the problem well posed.

The Method of Lagrange Multipliers

$$\text{Loss}(\mathbf{w}) = \mathbf{C} - \mathbf{w}\Sigma\mathbf{w}^\top$$



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Convert a **constrained optimization** into an **unconstrained optimization problem** by introducing the **Lagrangian**:

$$\mathcal{L}(\mathbf{w}, \lambda) = \text{Loss}(\mathbf{w}) + \lambda(\mathbf{w}\mathbf{w}^\top - 1)$$

The term $(\mathbf{w}\mathbf{w}^\top - 1)$ measures how much the **orthonormality constraint** ($\mathbf{w}\mathbf{w}^\top = 1$) is violated.

The **Lagrange multiplier** λ is chosen automatically by applying the **stationary point method** to the **Lagrangian**

- Differentiating with respect to $\mathbf{w}$:

$$\nabla_{\mathbf{w}}\text{Loss}(\mathbf{w}) + \lambda\nabla_{\mathbf{w}}(\mathbf{w}\mathbf{w}^\top - 1) = 0 \quad \Rightarrow \quad \nabla_{\mathbf{w}}\text{Loss}(\mathbf{w}) = -\lambda\nabla_{\mathbf{w}}(\mathbf{w}\mathbf{w}^\top - 1)$$

- Differentiating with respect to λ :

$$\frac{\partial}{\partial \lambda}\mathcal{L}(\mathbf{w}, \lambda) = (\mathbf{w}\mathbf{w}^\top - 1) = 0 \quad \Rightarrow \quad \mathbf{w}\mathbf{w}^\top = 1$$

Gradients of the **loss** and **scaled constraint violation** should be parallel!



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A Small Example

Minimize $f(x, y) = x + y$ subject to $x^2 + y^2 = 1$

$$\mathcal{L}(x, y, \lambda) = x + y + \lambda(x^2 + y^2 - 1)$$

$$\frac{\partial \mathcal{L}}{\partial x} = 1 + 2\lambda x = 0$$

$$\frac{\partial \mathcal{L}}{\partial y} = 1 + 2\lambda y = 0$$

so $x = y$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = x^2 + y^2 - 1 = 0$$

with $x = y$ this gives

$$x = y = \pm 1/\sqrt{2}$$

The minimum is $x = y = -1/\sqrt{2}$.

Applying the Method of Lagrange Multipliers



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Constructing the **Lagrangian**:

$$\text{Loss}(\mathbf{w}) = \mathbf{C} - \mathbf{w}\Sigma\mathbf{w}^\top$$

$$\mathcal{L}(\mathbf{w}, \lambda) = \mathbf{C} - \mathbf{w}\Sigma\mathbf{w}^\top + \lambda(\mathbf{w}\mathbf{w}^\top - 1)$$

Differentiating with respect to $\mathbf{w}$:

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}, \lambda) = -\nabla_{\mathbf{w}}\mathbf{w}\Sigma\mathbf{w}^\top + \lambda\nabla_{\mathbf{w}}(\mathbf{w}\mathbf{w}^\top - 1) = -\nabla_{\mathbf{w}}\mathbf{w}\Sigma\mathbf{w}^\top + \lambda\nabla_{\mathbf{w}}\mathbf{w}\mathbf{w}^\top$$

Compute the gradient of $\mathbf{w}\Sigma\mathbf{w}^\top$ by taking the partial derivatives:

$$\frac{\partial}{\partial w_i}\mathbf{w}\Sigma\mathbf{w}^\top = \frac{\partial}{\partial w_i}\sum_{j=1}^d\sum_{k=1}^dw_j\Sigma_{jk}w_k = \sum_{j=1}^dw_j\Sigma_{ji} + \sum_{k=1}^d\Sigma_{ik}w_k$$

$$\nabla_{\mathbf{w}}\mathbf{w}\Sigma\mathbf{w}^\top = \Sigma\mathbf{w}^\top + \Sigma^\top\mathbf{w}^\top = (\underbrace{\Sigma + \Sigma^\top})\mathbf{w}^\top = 2\Sigma\mathbf{w}^\top$$

Doing the same for $\nabla_{\mathbf{w}}\mathbf{w}\mathbf{w}^\top$ we obtain:

$\Sigma = \mathbf{X}^\top\mathbf{X}$ is symmetric

$$\nabla_{\mathbf{w}}\mathcal{L}(\mathbf{w}, \lambda) = -2\Sigma\mathbf{w}^\top + 2\lambda\mathbf{w}^\top$$



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Differentiating with respect to $\mathbf{w}$:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = -\nabla_{\mathbf{w}} \mathbf{w} \Sigma \mathbf{w}^{\top} + \lambda \nabla_{\mathbf{w}} (\mathbf{w} \mathbf{w}^{\top} - 1) = -\nabla_{\mathbf{w}} \mathbf{w} \Sigma \mathbf{w}^{\top} + \lambda \nabla_{\mathbf{w}} \mathbf{w} \mathbf{w}^{\top}$$

Compute the gradient of $\mathbf{w} \Sigma \mathbf{w}^{\top}$ by taking the partial derivatives:

$$\frac{\partial}{\partial w_i} \mathbf{w} \Sigma \mathbf{w}^{\top} = \frac{\partial}{\partial w_i} \sum_{j=1}^d \sum_{k=1}^d w_j \Sigma_{jk} w_k = \sum_{j=1}^d w_j \Sigma_{ji} + \sum_{k=1}^d \Sigma_{ik} w_k$$

$$\nabla_{\mathbf{w}} \mathbf{w} \Sigma \mathbf{w}^{\top} = \Sigma \mathbf{w}^{\top} + \Sigma^{\top} \mathbf{w}^{\top} = \underbrace{(\Sigma + \Sigma^{\top})}_{\Sigma = \mathbf{X}^{\top} \mathbf{X} \text{ is symmetric}} \mathbf{w}^{\top} = 2 \Sigma \mathbf{w}^{\top}$$

Doing the same for $\nabla_{\mathbf{w}} \mathbf{w} \mathbf{w}^{\top}$ we obtain:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = -2 \Sigma \mathbf{w}^{\top} + 2 \lambda \mathbf{w}^{\top}$$

Setting $\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \lambda) = 0$ we obtain a key result:

$$\Sigma \mathbf{w}^{\top} = \lambda \mathbf{w}^{\top}$$



What is this?



What does this equation
 $(\Sigma \mathbf{w}^T = \lambda \mathbf{w}^T)$ say about $\mathbf{w}$?



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The Eigenvector Equation

Therefore, we know that $\mathbf{w}^*$ must be an eigenvector.

$$\Sigma \mathbf{w}^\top = \lambda \mathbf{w}^\top$$

It must also be **unit length** to satisfy the $\mathbf{w}\mathbf{w}^\top = 1$ constraint.

If we return to the original loss definition and substitute $\Sigma \mathbf{w}^\top = \lambda \mathbf{w}^\top$

$$\text{Loss}(\mathbf{w}) = -\mathbf{w}\Sigma \mathbf{w}^\top = -\mathbf{w}(\lambda \mathbf{w}^\top) = -\lambda \mathbf{w}\mathbf{w}^\top = -\lambda$$

We see that $\mathbf{w}^*$ must be the Eigenvector with the **largest Eigenvalue**.

The **first principal component** is the **unit eigenvector** of $\Sigma = \mathbf{X}^\top \mathbf{X}$ associated with the **largest eigenvalue**.



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Subsequent Principal Components

Repeating for the next principal component $\mathbf{w}_2$, with one additional constraint:

$$\mathbf{w}_2 \mathbf{w}_1^\top = \mathbf{0}$$

This introduces an additional Lagrange multiplier.

$$\mathcal{L}(\mathbf{w}_2, \lambda_2, \gamma) = -\mathbf{w}_2 \mathbf{\Sigma} \mathbf{w}_2^\top + \lambda_2 (\mathbf{w}_2 \mathbf{w}_2^\top - 1) + \gamma (\mathbf{w}_2 \mathbf{w}_1^\top)$$

Differentiating with respect to $\mathbf{w}_2$ and left multiply by $\mathbf{w}_1$ you can show that $\gamma = 0$ and again (*try doing this yourself*):

$$\mathbf{\Sigma} \mathbf{w}_2^\top = \lambda_2 \mathbf{w}_2^\top$$

Hence $\mathbf{w}_2$ is the eigenvector associated with the second largest eigenvalue.

The rows of $\mathbf{W}$ are the **leading k eigenvectors** of $\mathbf{\Sigma}$, and the **latent factors (coordinates)** are:

$$\mathbf{Z} = \mathbf{XW}^\top$$



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Computing the Principal Components

Constructing $\mathbf{X}^\top \mathbf{X}$ and computing its eigen decomposition is correct but expensive.

Instead, we typically use the **singular value decomposition**:

$$\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^\top$$

```
U, S, Vt = np.linalg.svd(X, full_matrices=False)
```

The columns of $\mathbf{V}$ are precisely the eigenvectors of $\mathbf{X}^\top \mathbf{X}$.

- *This result is stated without proof today (but you can do it for homework). The [EECS 16B notes on the SVD](#) are a great reference, and [Steve Brunton's video series on the PCA](#) is excellent.*



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Returning to the vote data

Given the singular value decomposition $\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^\top$.

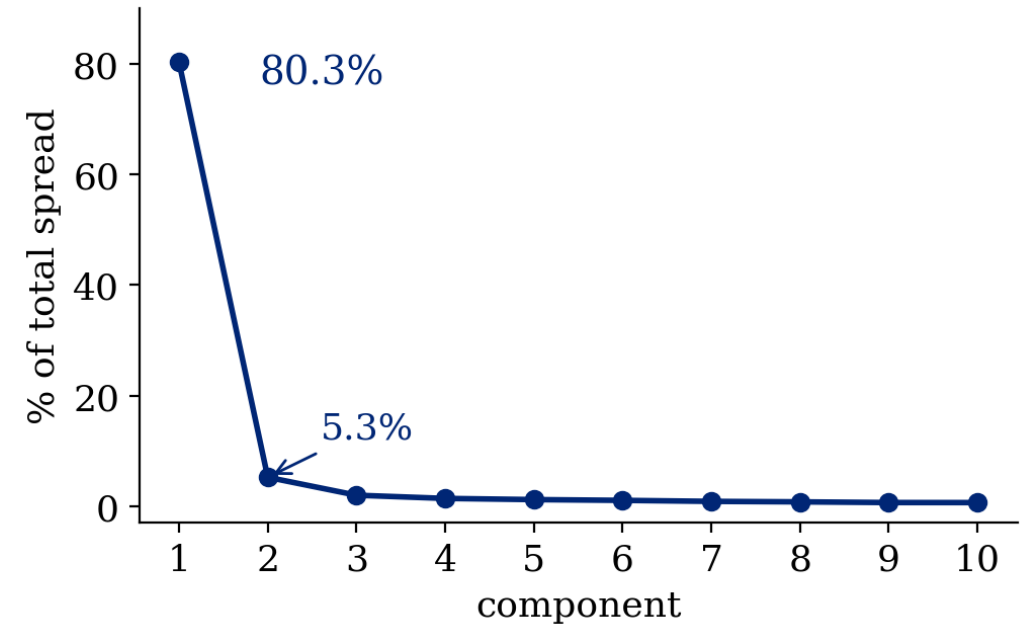
The **Explained Variance Ratio** is

$$\frac{s_{ii}^2}{\sum_{d=1}^d s_{dd}^2}$$

the share of the **total spread** accounted for by each principal component.

PC1: 80.3% PC2: 5.3% together: 85.6%

- The **sharp decrease** after the first component is what makes the two-dimensional plot trustworthy.
- The centered matrix nonetheless has full rank 41. The data is **approximately two-dimensional**.



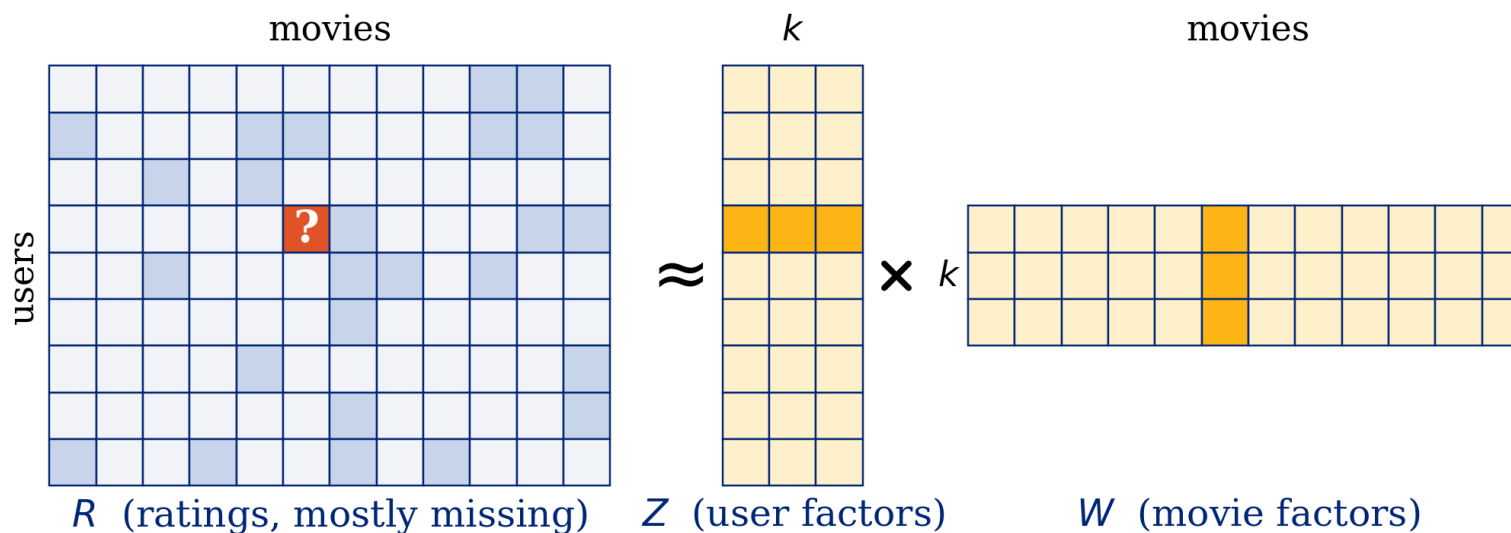
Bonus

Matrix Factorization for Content Recommendation



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- **R holds ratings:** one row per user, one column per movie, and almost every entry is missing
- **Netflix Prize:** 8.5 billion user and movie pairs, of which about 1 in 85 was ever rated



A missing rating is predicted by the dot product of that user's row with that movie's column

$$\text{Loss}(Z, W) = \sum_{(i,j) \in \Omega} (R_{ij} - Z_i W_j)^2 + \alpha (\|Z\|^2 + \|W\|^2)$$

Drop unit vector constraint and add a **penalty term**.

Only the **observed pairs** Ω are part of the loss.
The **learned factors** are then used to **fill in every rating** that was never given.

Summary



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- **Dimensionality reduction** was posed as a **factorization**,
$$\mathbf{X} \approx \mathbf{Z} \mathbf{W}$$
- Optimality was defined as **smallest reconstruction error**, which proved equivalent to greatest spread
- Applied **stationary point method** to optimize the loss:
 - Differentiating with respect to $\mathbf{z}$ showed that the **optimal coefficient** is a **projection**
 - Differentiating with respect to $\mathbf{w}$, subject to a constraint, produced an **eigenvector problem**
- The principal components are the **leading eigenvectors** of $\frac{1}{n} \mathbf{X}^\top \mathbf{X}$, and the **latent factors (coordinates)** are the **projections** $\mathbf{Z} = \mathbf{X} \mathbf{W}^\top$

Next week we turn to probability!

Lecture 3

Dimensionality Reduction

Credit: Joseph E. Gonzalez and Narges Norouzi

Reference Book Chapters:

- **Linear Algebra, Matrix Calculus, and Eigenvectors:** Appendix (A.1, A.3, A.4)
- **Lagrange Multipliers:** Appendix C
- **PCA:** Chapter 16.1

Have Fun!!!