# Dimensionality Reduction

Lecture 12

# The Curse of Dimensionality

# Challenge 1

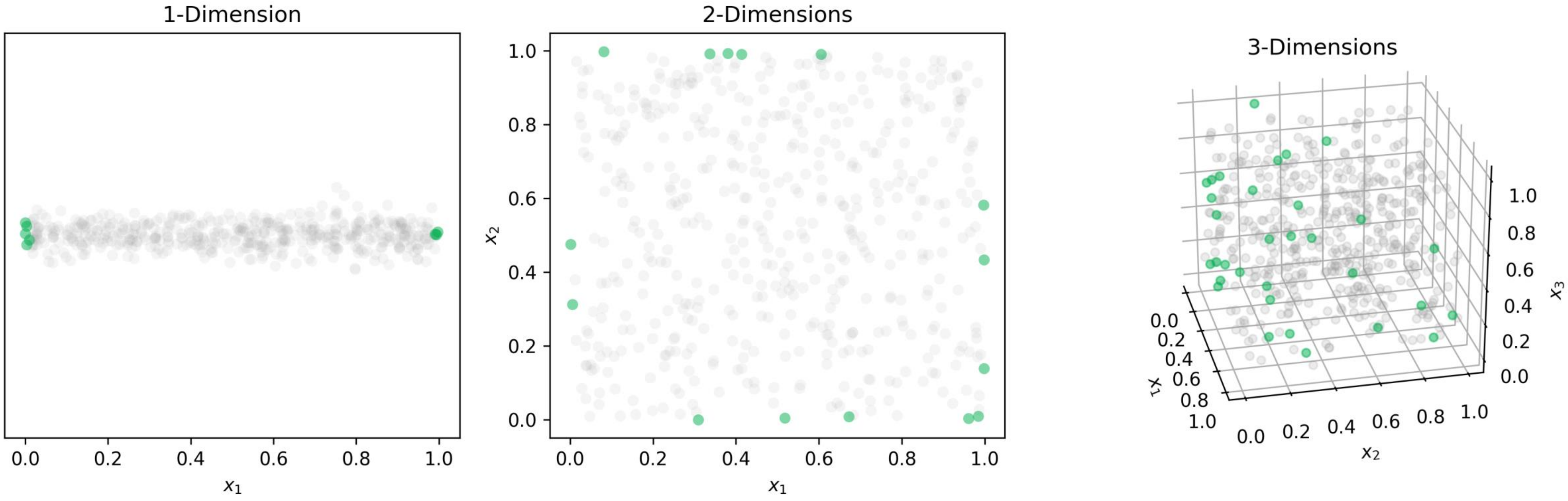
**In high dimensions, data become sparse**

(increasing the risk of overfitting)

# Random data points in a unit hypercube…

Data point is a distance < 0.01 units from the edge of a unit hypercube

All other data



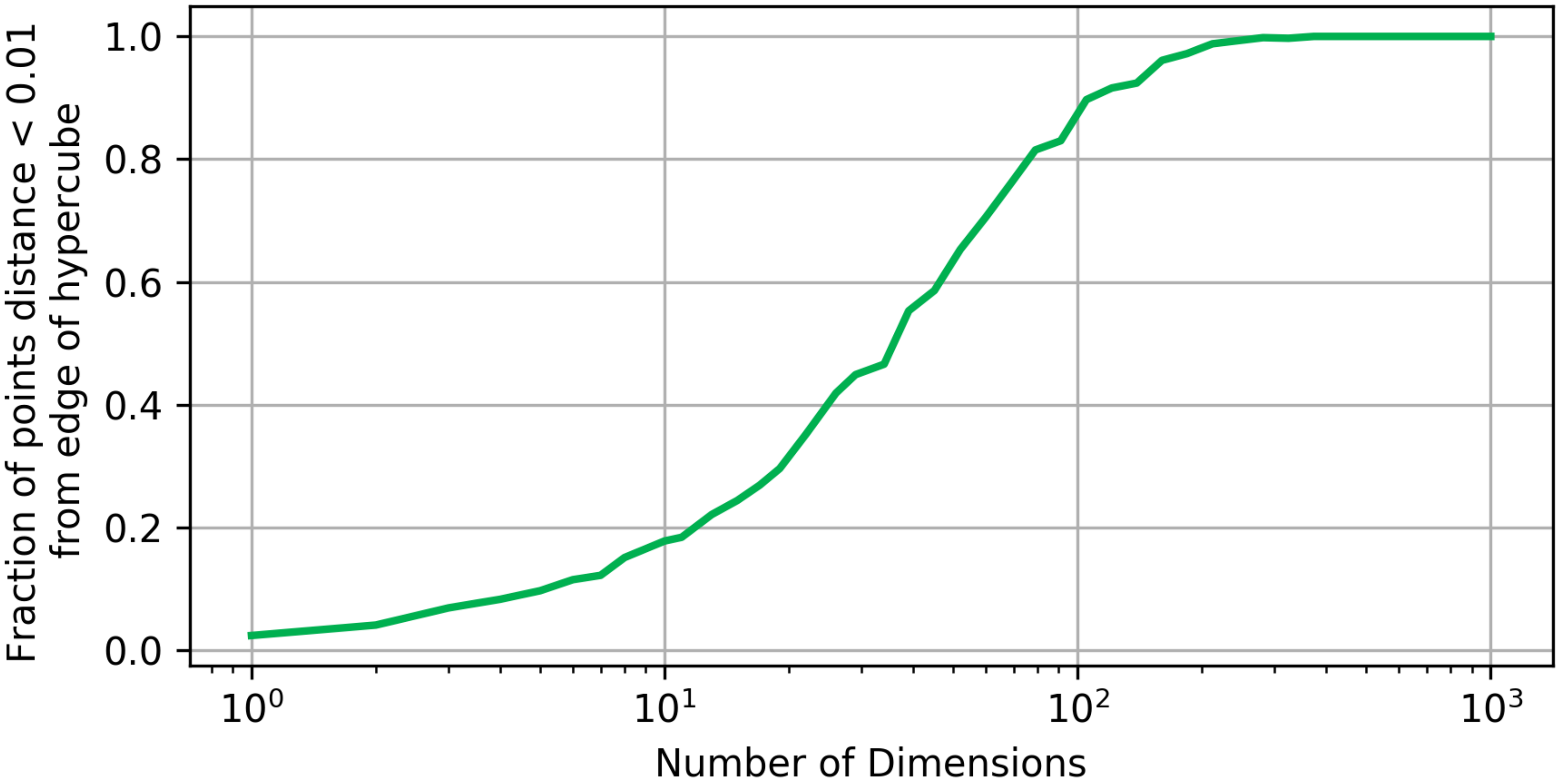

Fraction of edge data = 

0.016

0.030

0.064

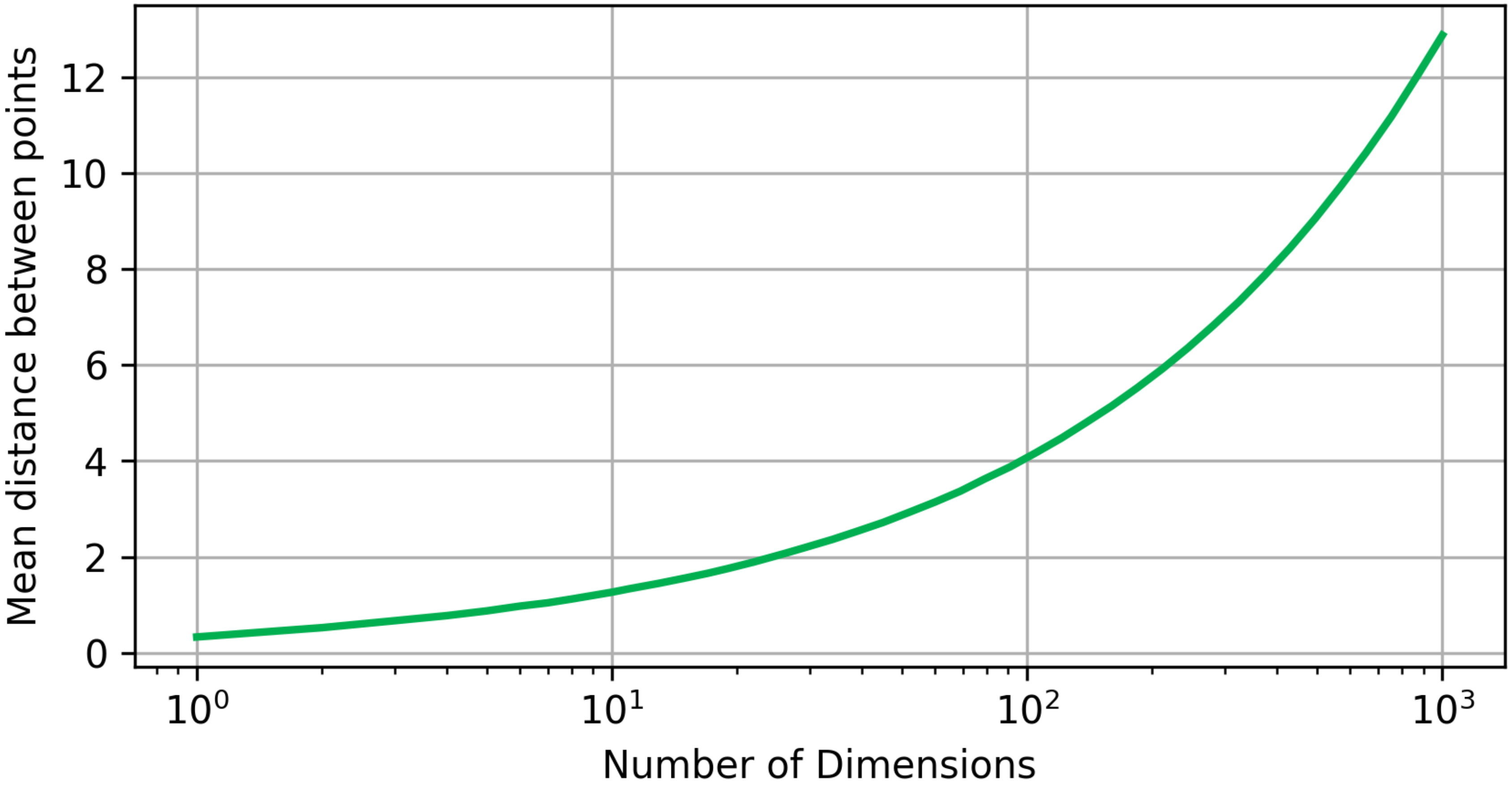
# In high dimensions…




…nearly all of the high dimensional space is **far away from the center**

Note: figures constructed using 1,000 random points

# In high dimensions…




…data become sparse

Note: figures constructed using 1,000 random points

# Challenge 2

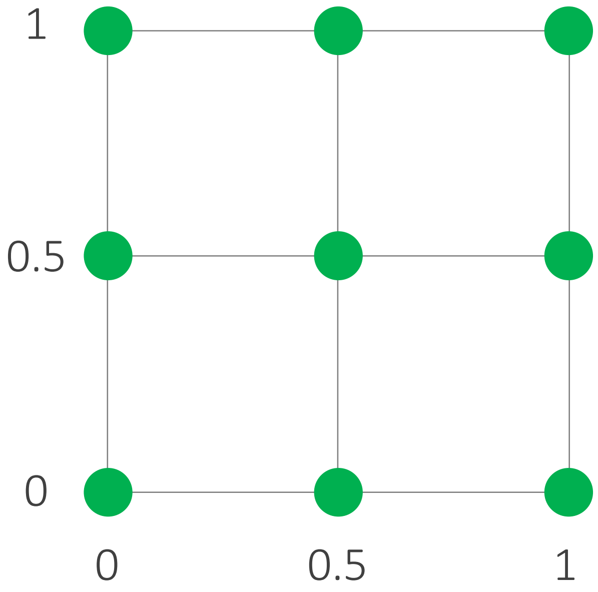
**Much more data are needed for sampling higher dimensional spaces**

# Sample a unit hypercube on a grid spaced at intervals of 0.5

**D = 1**

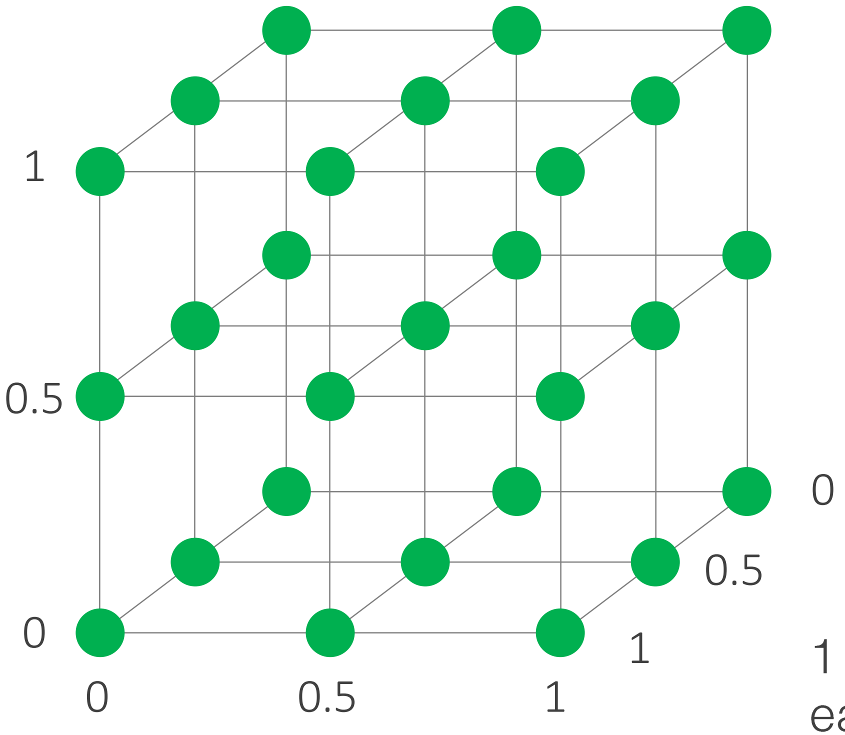

**N = 3**

**D = 2**




**N = 9**

**D = 3**




**N = 27**

| Dim (D) | Samples (N) |
|---|---|
| 4 | 81 |
| 5 | 243 |
| 10 | 59,049 |
| 100 | $5.2 \times 10^{47}$ |
| **300** | $\mathbf{1.4 \times 10^{143}}$ |

1 million Googles, each with 20 exabytes of data would only be $10^{25}$ bytes

**…it takes more data to learn in high dimensional spaces**

# Dimensionality Reduction

## Benefits:

Simplified computation
Reduced redundancy of features
Improved numerical stability due to removed correlations

## Popular approach:

Principal Components Analysis (PCA)

# PCA

**Before you begin: Normalize the data!**

For each feature, subtract the mean and divide by the standard deviation

Normalized feature

Raw, unscaled feature

$$x = \frac{x' - \overline{x'}}{\sigma_{x'}}$$

$$\begin{array}{cc} & \text{columns = features} \\ \mathbf{X} = & \begin{bmatrix} x_{11} & \cdots & x_{1D} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{ND} \end{bmatrix} \text{rows = observations} \end{array}$$

We normalize each of the columns

# Principal components analysis

a.k.a.
Karhunen–Loève Transform
Proper orthogonal decomposition
Hotelling transform

Transform the data from a high dimensional space to a lower dimensional subspace, while minimizing the projection error

$$\mathrm{A} \qquad \mathbf{x} \rightarrow \mathbf{z}$$

$$\mathbb{R}^{M\times D} \qquad \mathbb{R}^{D} \qquad \mathbb{R}^{M} \qquad M < D$$

$$\begin{bmatrix} u_{11} & \cdots & u_{1D} \\ \vdots & \ddots & \vdots \\ u_{M1} & \cdots & u_{MD} \end{bmatrix} \qquad \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_D \end{bmatrix} \qquad \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_M \end{bmatrix}$$

linear transformation matrix
(this is what we want to find through PCA)

sample of data in original D-dimensional space
(this is one of N observations)

Transformed data in M-dimensional (lower dimensional) subspace

# Principal components analysis

$$A$$

$$\begin{bmatrix} u_{11} & \cdots & u_{1D} \\ \vdots & \ddots & \vdots \\ u_{M1} & \cdots & u_{MD} \end{bmatrix} = \begin{bmatrix} - & \mathbf{u}_1^T & - \\ & \vdots & \\ - & \mathbf{u}_M^T & - \end{bmatrix}$$

linear transformation matrix

Each $\mathbf{u}_i$ represents a unit vector

The $i^{\text{th}}$ principal component:

$$\underbrace{z_i}_{\text{scalar}} = \underbrace{\mathbf{u}_i^T}_{\text{unit vector}} \mathbf{x}$$

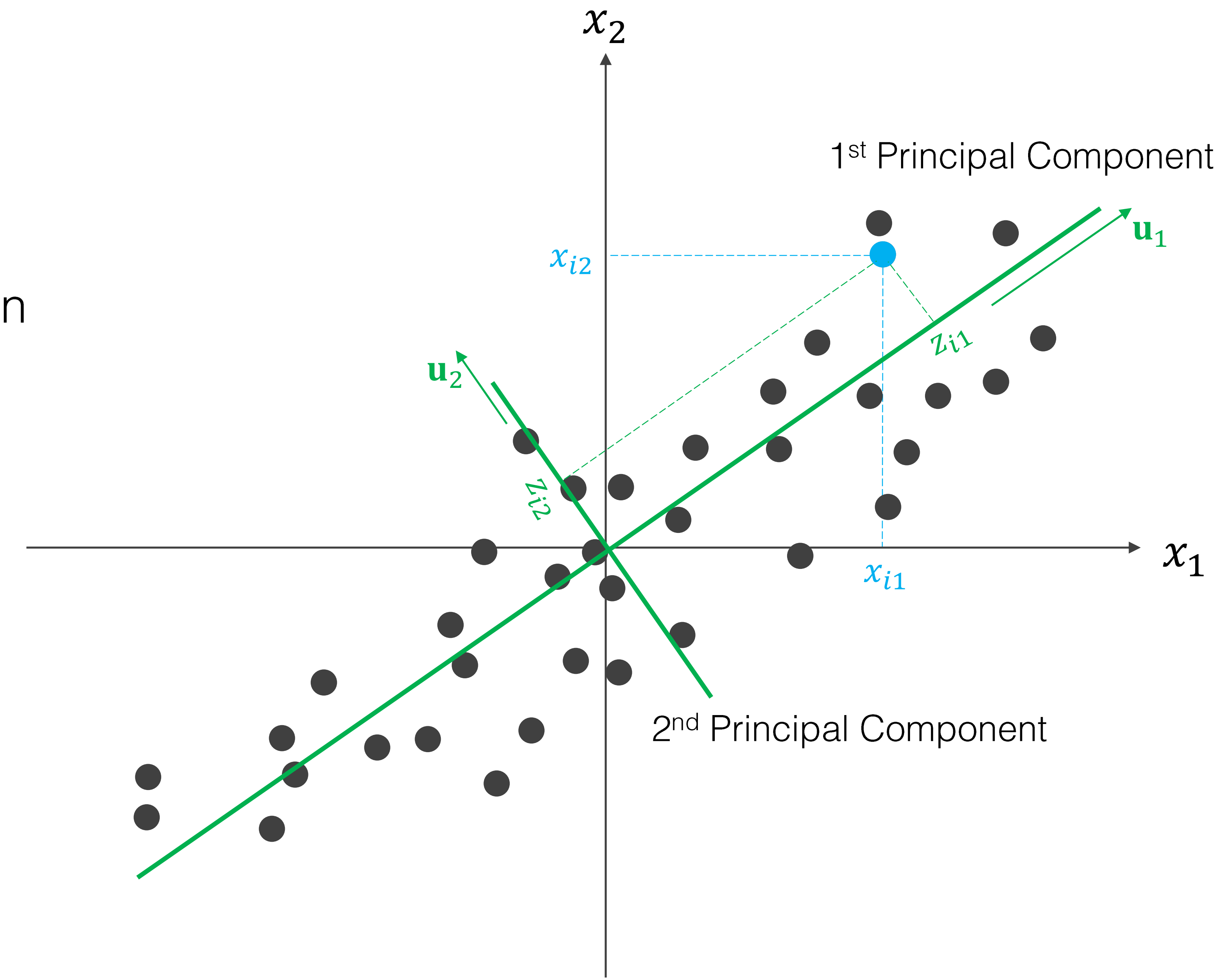
Since only direction matters, we assume the $\mathbf{u}_i$ are unit vectors

$$\mathbf{u}_i^T \mathbf{u}_i = 1$$

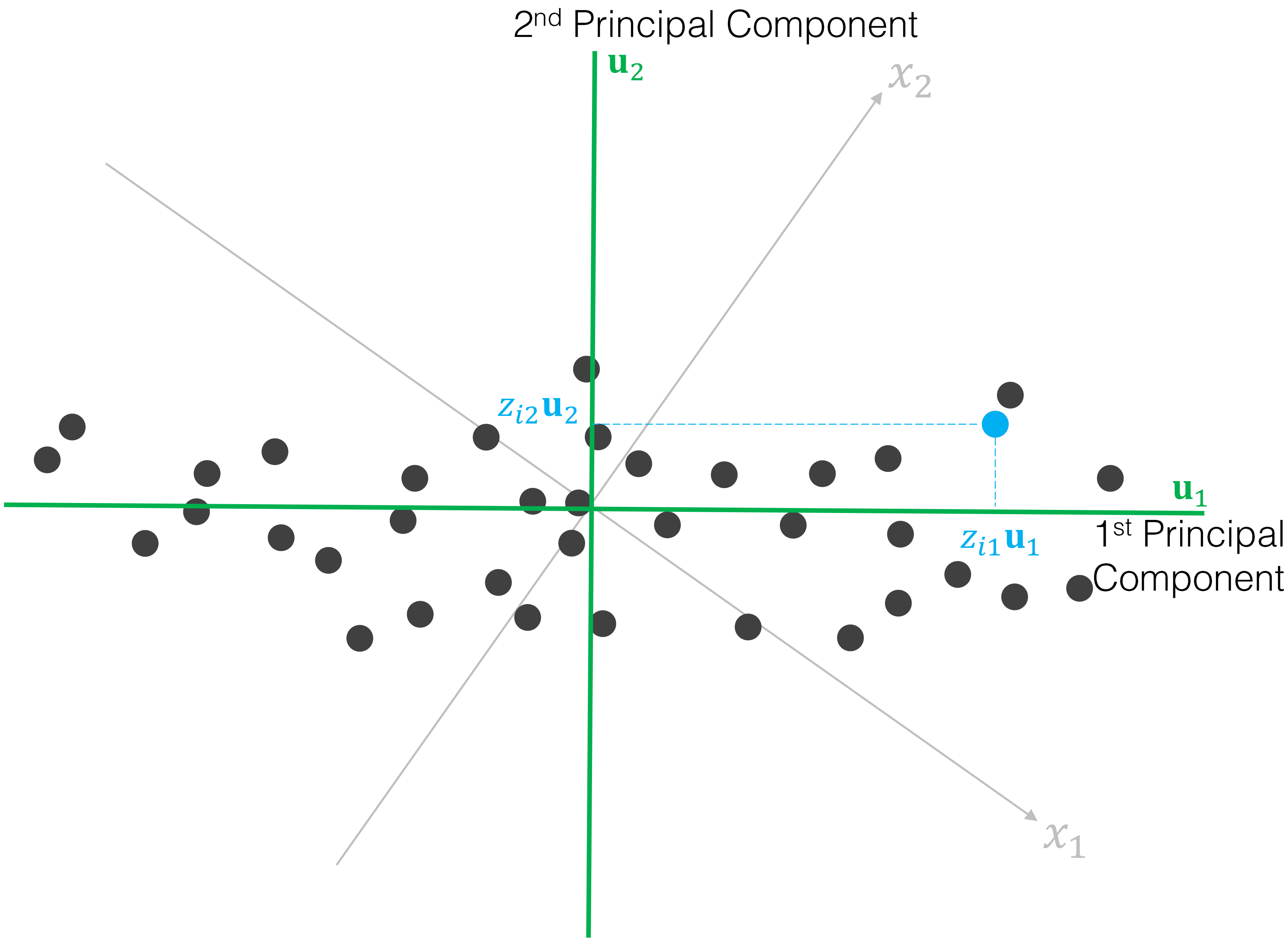
# Principal Components

Maximum variance formulation

$$\mathbf{x}_i = \begin{bmatrix} x_{i1} \\ x_{i2} \end{bmatrix}$$



# Reprojected Data onto Principal Components




Any point $\boldsymbol{x}_i$ can be represented as a combination of the principle components

$$\mathbf{x}_i = \sum_{j=1}^{D} z_{ij}\mathbf{u}_j$$

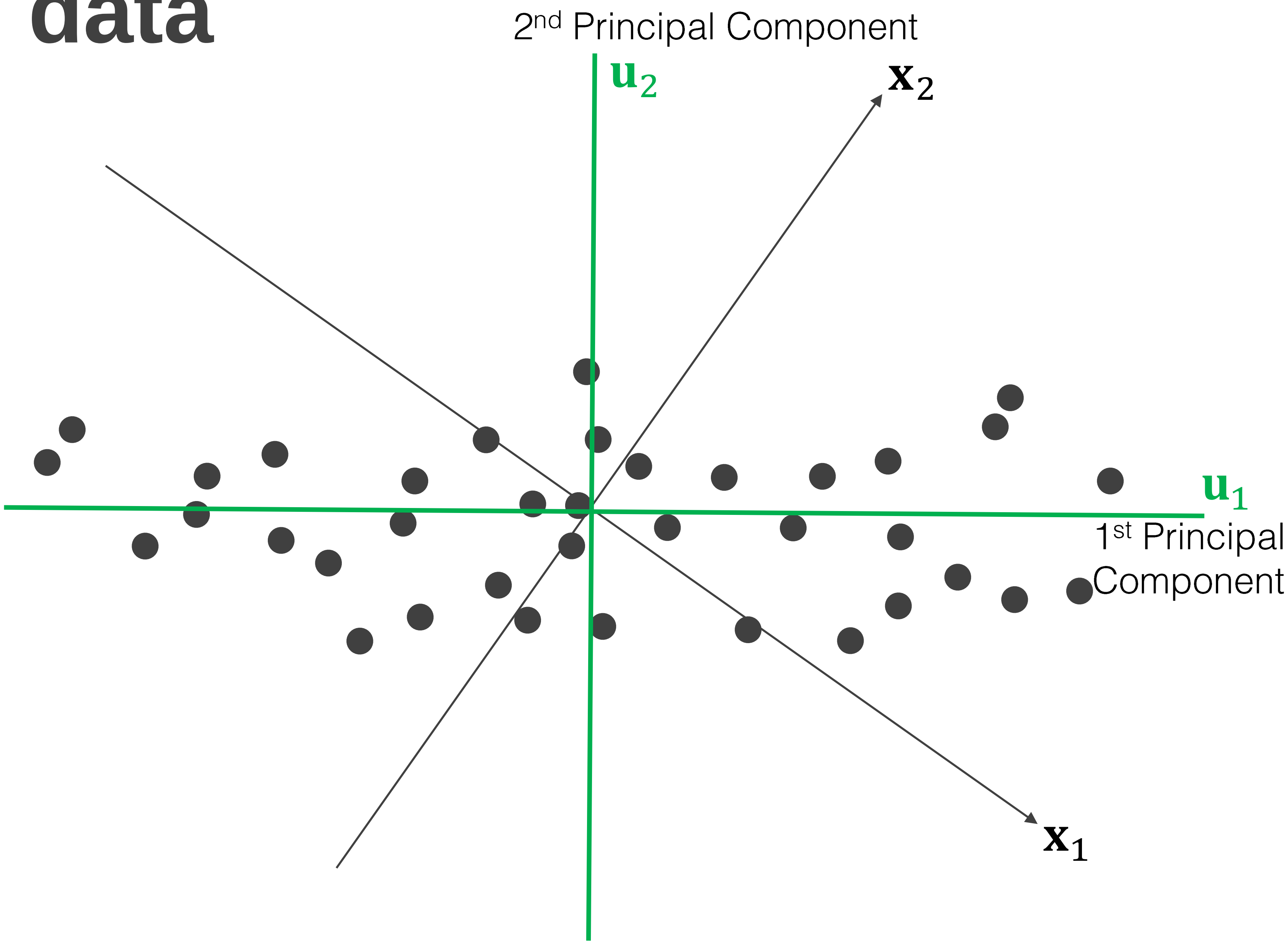
The $\mathbf{u}_j$'s are an orthogonal basis for the space $\mathbb{R}^D$

# Approximating data with principal components

scalar projection

principal component direction

$$\mathbf{x}_j = \sum_{i=1}^{D} (\mathbf{x}_j^T \mathbf{u}_i)\mathbf{u}_i$$



# PCA

We want to **maximize the variance** of the projected data

Goal

Let's start by finding the **unit vector in the direction of greatest variation** in the dataset

Here the magnitude is unimportant, but the direction matters

We seek to project each point $\boldsymbol{x}_i$ onto a unit PC vector. $z_i = \boldsymbol{u}_1^T \boldsymbol{x}_i$

# PCA: Compute the variance of the transformed data

Mean of the data:

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}_i \qquad \mathbf{x}_i \; [D \times 1]$$

The projected mean of the data:

$$\bar{z} = \mathbf{u}_1^T \, \bar{\mathbf{x}}$$

We can compute the sample variance as:

$$\underset{[\text{scalar}]}{\sigma_z^2} = \frac{1}{N}\sum_{i=1}^{N} (z_i - \bar{z})^2$$

$$\sigma_z^2 = \frac{1}{N}\sum_{i=1}^{N} (\mathbf{u}_1^T \mathbf{x}_i - \mathbf{u}_1^T \bar{\mathbf{x}})^2$$

The magnitude $z_i$ of our data $\mathbf{x}_i$ projected onto the unit vector $\mathbf{u}_1$ is:

$$z_i = \mathbf{u}_1^T \, \mathbf{x}_i$$

# PCA: Compute the variance of the transformed data

We can compute the sample variance as:

$$\sigma_z^2 = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{u}_1^T\mathbf{x}_i - \mathbf{u}_1^T\bar{\mathbf{x}})^2$$

$$= \frac{1}{N}\sum_{i=1}^{N}\mathbf{u}_1^T(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T\mathbf{u}_1$$

$$= \mathbf{u}_1^T\boldsymbol{\Sigma}\mathbf{u}_1$$

Variance of the projected data

Define:

$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

Covariance matrix of our data

# Covariance matrix

$$\mathbf{x}_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{iD} \end{bmatrix}$$

Vector of observation $i$

$x_{ij}$

Observation index

Predictor index

Predictors →

$$\mathbf{X} = \begin{array}{c} \text{Observations} \end{array} \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T \rightarrow [D \times D]$$

$$[D \times 1][1 \times D]$$

Mean of each predictor

If $\mu_j = 0$ for all $j$

This will be the case IF the data are standardized

$$\boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} & \cdots & \Sigma_{1D} \\ \Sigma_{21} & \Sigma_{22} & \cdots & \Sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{D1} & \Sigma_{D2} & \cdots & \Sigma_{DD} \end{bmatrix}$$

$$\Sigma_{jk} = \frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

$$= \mathrm{cov}(X_j, X_k)$$

$$= E[(X_j - \mu_j)(X_k - \mu_k)]$$

$$\Sigma_{jk} = \frac{1}{N}\sum_{i=1}^{N} x_{ij}x_{ik}$$

$$= \frac{1}{N}\mathbf{x}_j^T\mathbf{x}_k$$

$$= E[X_j X_k]$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \Sigma_{12} & \cdots & \Sigma_{1D} \\ \Sigma_{21} & \sigma_2^2 & \cdots & \Sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{D1} & \Sigma_{D2} & \cdots & \sigma_D^2 \end{bmatrix}$$

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \bar{x}_j)^2$$

$$= E[(X_j - \mu_j)^2]$$

$$\boldsymbol{\Sigma} = \frac{1}{N}\mathbf{X}^{\mathrm{T}}\mathbf{X}$$

# Covariance matrix properties

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \Sigma_{12} & \cdots & \Sigma_{1D} \\ \Sigma_{21} & \sigma_2^2 & \cdots & \Sigma_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ \Sigma_{D1} & \Sigma_{D2} & \cdots & \sigma_D^2 \end{bmatrix}$$

Positive semidefinite ($\boldsymbol{v}^T \boldsymbol{\Sigma} \boldsymbol{v} \geq 0$ for all $\boldsymbol{v}$) and symmetric ($\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{\mathrm{T}}$)

All eigenvalues are positive

Eigenvectors are orthogonal

If the features (predictors), $x_1, x_2, \dots, x_D$ are independent, $\boldsymbol{\Sigma}$ is diagonal because $\mathrm{cov}(X_j, X_k) = 0$ if $j \neq k$

# PCA: Maximize the variance

We want to **maximize variance** $\sigma_z^2 = \mathbf{u}_1^T \boldsymbol{\Sigma} \mathbf{u}_1$

subject to $\mathbf{u}_1^T \mathbf{u}_1 = 1$ (unit vectors)

We can use **Lagrange multipliers**:

Maximize $f(x)$

subject to the constraint $g(x)$

We maximize this: $L(x, \lambda) = f(x) - \lambda g(x)$

$$f(\mathbf{x}, \mathbf{u}_i) = \mathbf{u}_1^T \boldsymbol{\Sigma} \mathbf{u}_1$$

$$g(\mathbf{x}, \mathbf{u}_i) = \mathbf{u}_1^T \mathbf{u}_1 - 1 = 0$$

For our case: $L(\mathbf{x}, \mathbf{u_1}, \lambda) = \mathbf{u}_1^{\mathrm{T}} \boldsymbol{\Sigma} \mathbf{u}_1 - \lambda(\mathbf{u}_1^T \mathbf{u}_1 - 1)$

We take the derivative and set it equal to zero

# PCA

$$L(\mathbf{x}, \mathbf{u_1}, \lambda) = \mathbf{u}_1^T \mathbf{\Sigma} \mathbf{u}_1 - \lambda(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

We take the derivative with respect to $\mathbf{u_1}$ and set it equal to zero

$$\frac{\partial L}{\partial \mathbf{u}_1} = \frac{\partial}{\partial \mathbf{u}_1} \mathbf{u}_1^T \mathbf{\Sigma} \mathbf{u}_1 - \frac{\partial}{\partial \mathbf{u}_1} \lambda(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

$$= 2\mathbf{\Sigma}\mathbf{u}_1 - 2\lambda\mathbf{u}_1 = 0$$ (since Σ is symmetric)

$$\mathbf{\Sigma}\mathbf{u}_1 = \lambda\mathbf{u}_1 \quad \rightarrow$$

$\mathbf{u}_1$ is an eigenvector of the covariance matrix $\mathbf{\Sigma}$, and $\lambda$ is an eigenvalue

How do we know which eigenvector to use as the first principal component?

# Eigenanalysis and PCA

Eigenvector Demo:

http://setosa.io/ev/eigenvectors-and-eigenvalues/

PCA Demo:

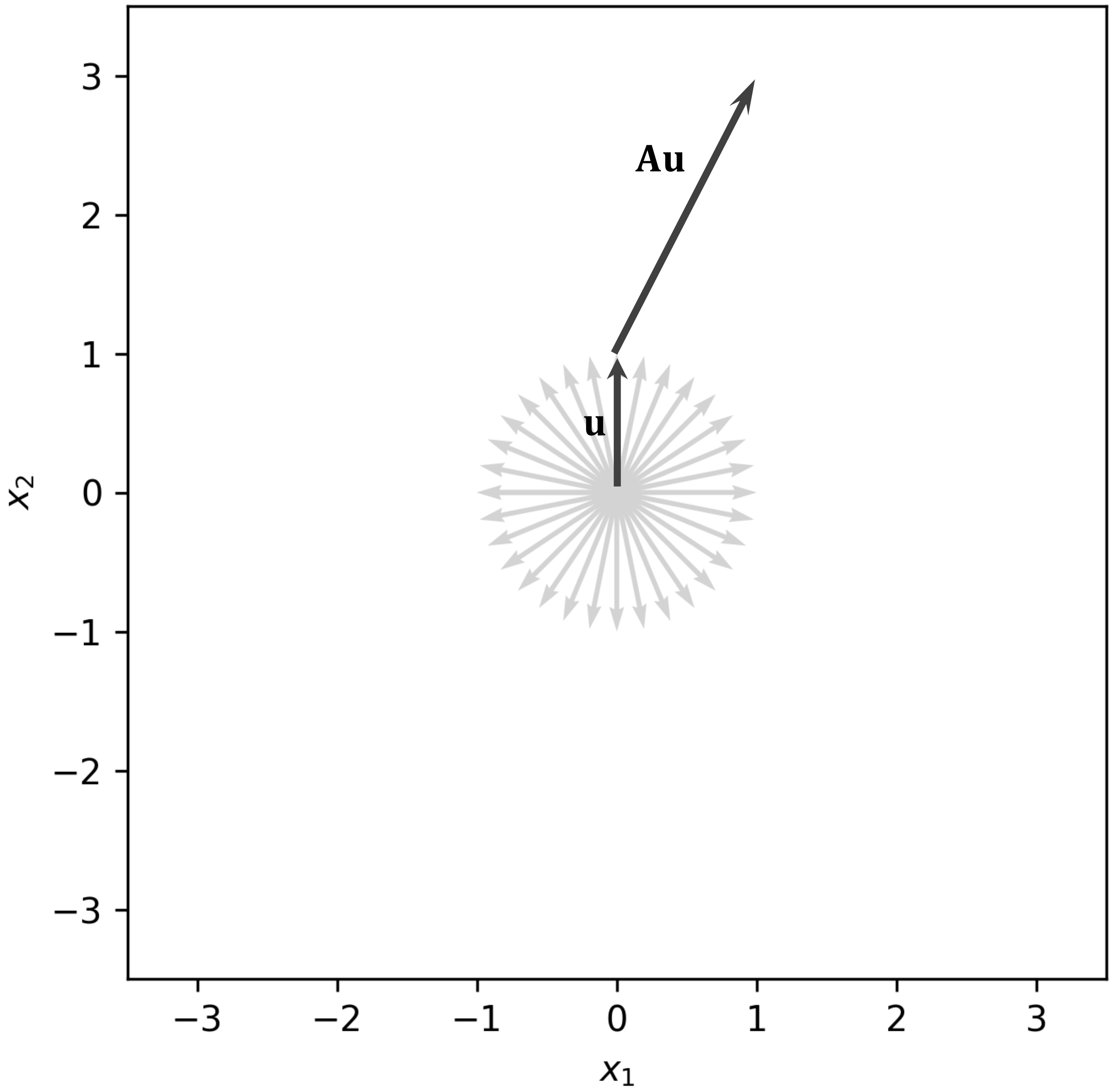
http://setosa.io/ev/principal-component-analysis/

# Eigenvalues/Eigenvectors

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

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\mathbf{v} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbf{A}\mathbf{v} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$



# Eigenvalues/Eigenvectors

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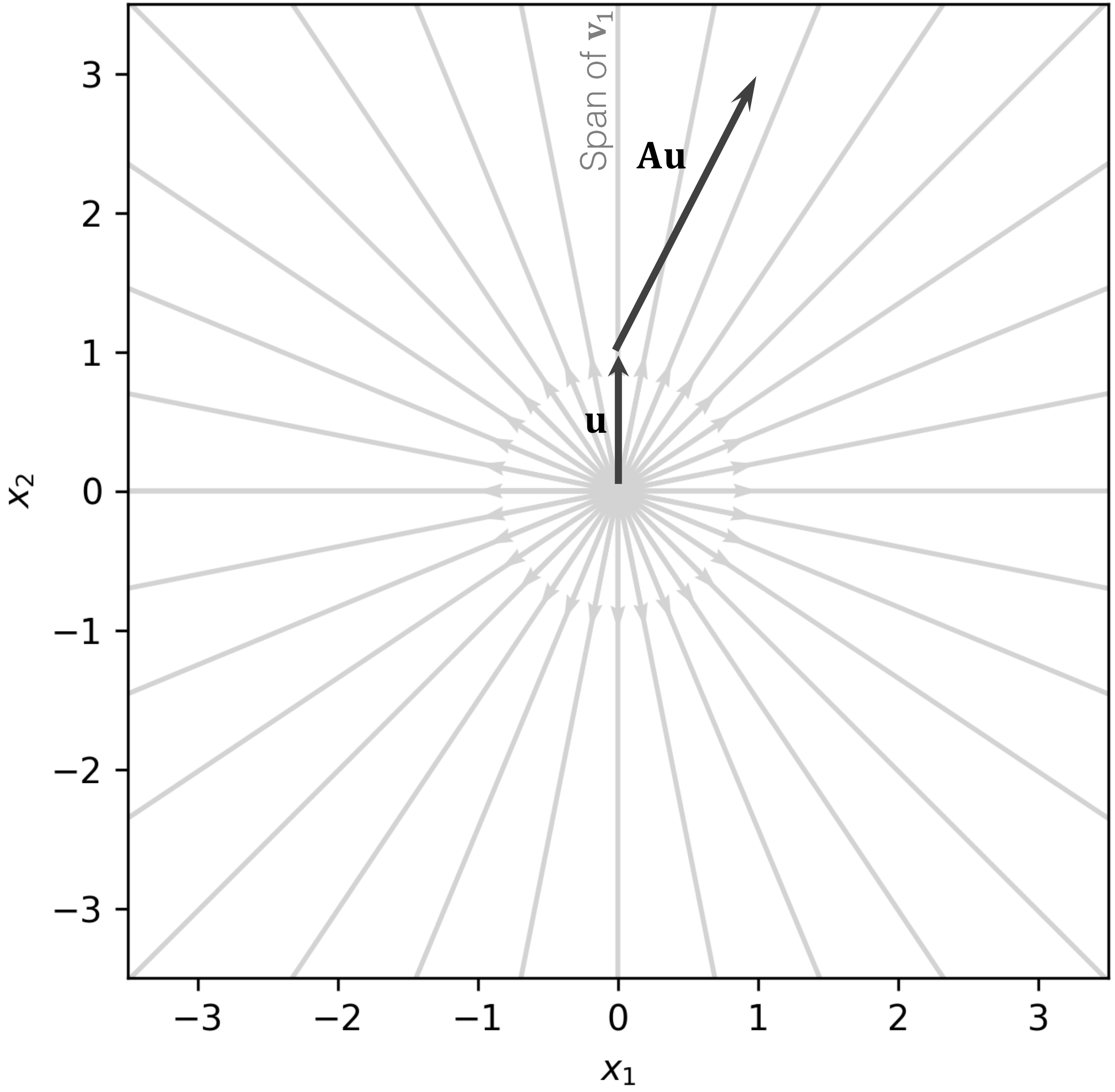
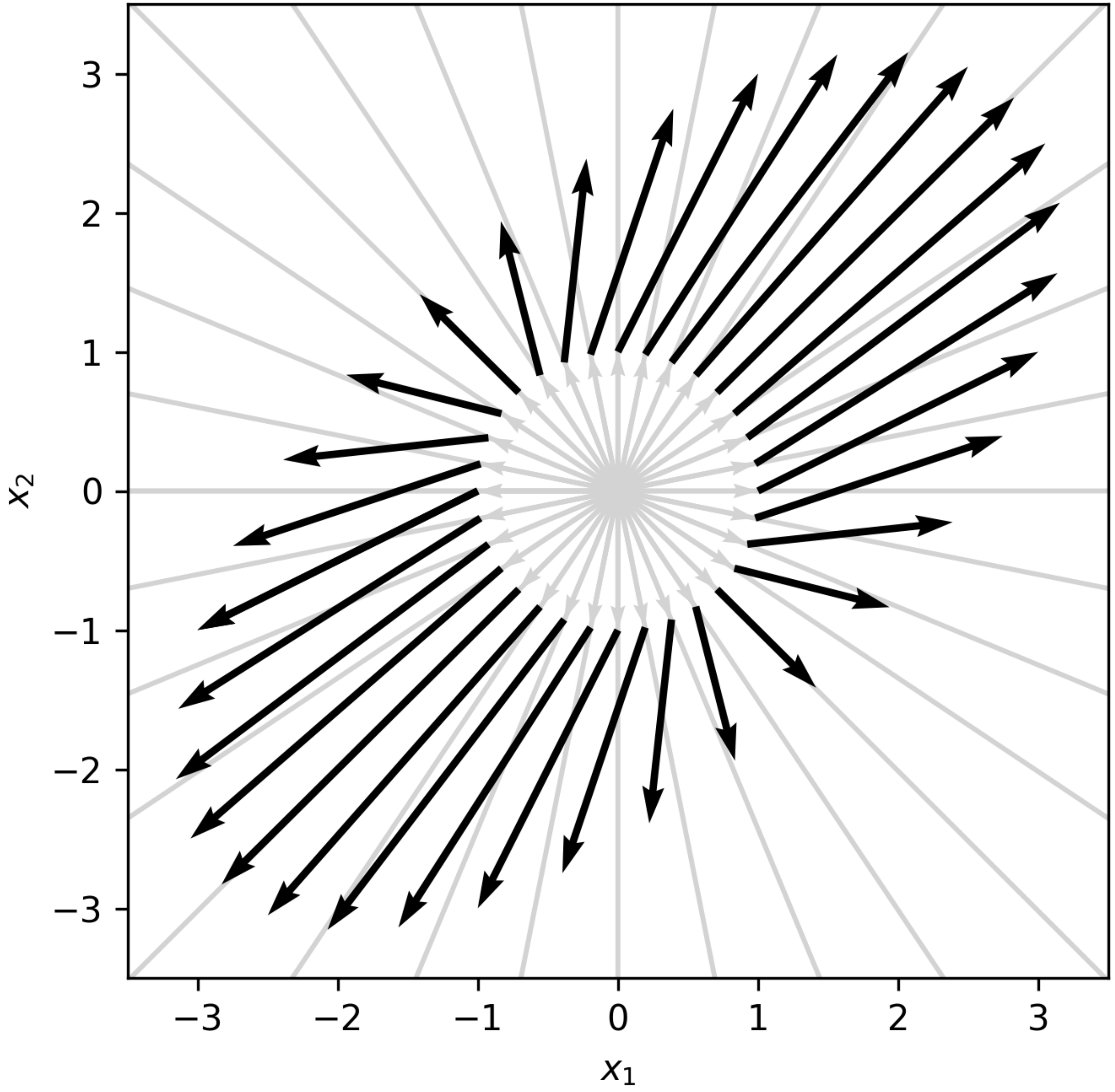


# Eigenvalues/Eigenvectors

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

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$



# Eigenvalues/Eigenvectors

$$\mathbf{Au} = \lambda \mathbf{u}$$

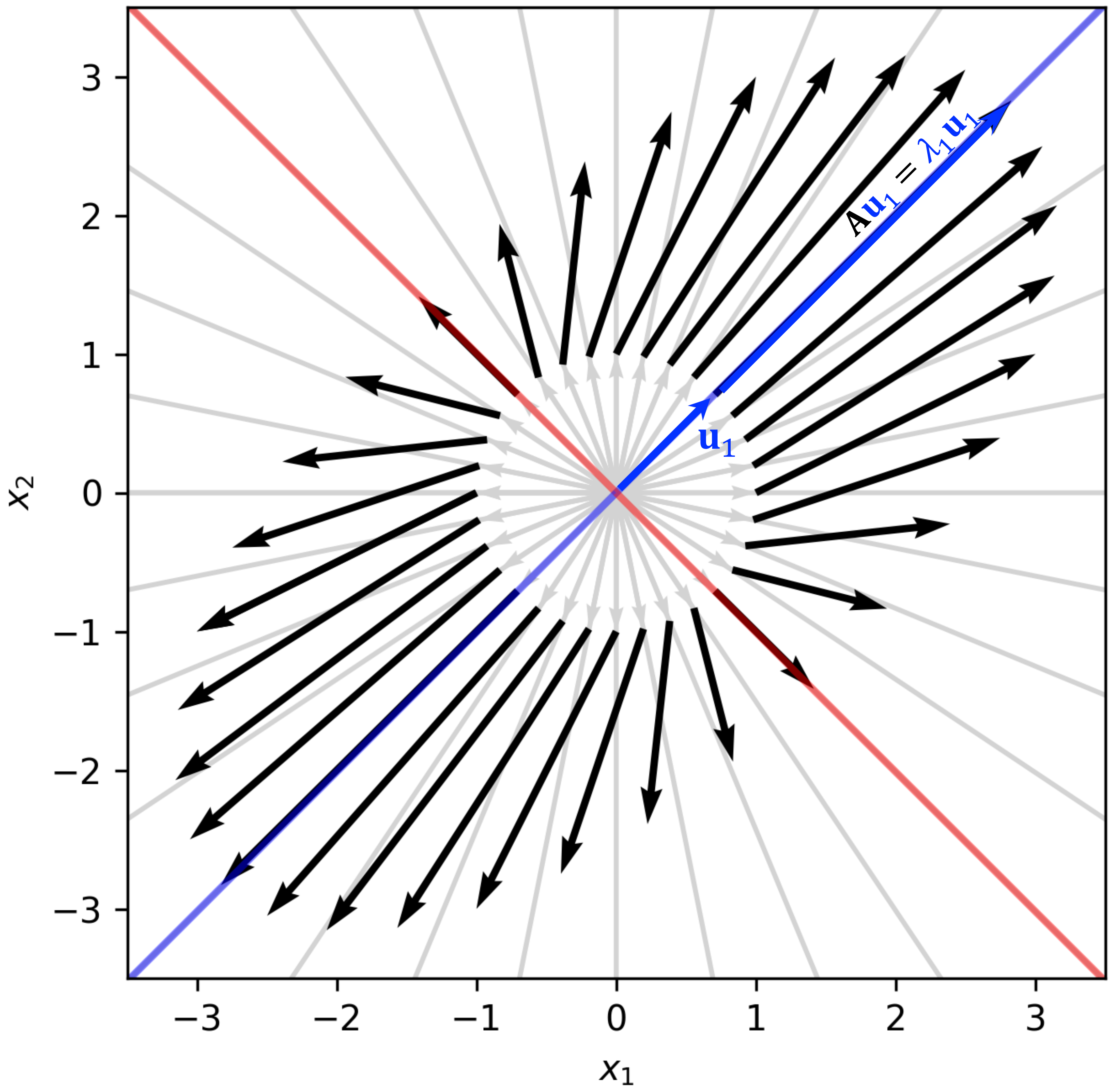
$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\mathbf{u}_1 = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix} \qquad \lambda_1 = 3$$

$$\mathbf{Au}_1 = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$

$$= \begin{bmatrix} 2.12 \\ 2.12 \end{bmatrix}$$

$$= \lambda_1 \mathbf{u}_1 = 3 \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$



# PCA

Since we want to maximize the variance in the projected features:

We want to maximize: $\sigma_z^2 = \mathbf{u}_1^T \boldsymbol{\Sigma} \mathbf{u}_1$

To do that this must be true: $\boldsymbol{\Sigma} \mathbf{u}_1 = \lambda \mathbf{u}_1$
(shown on last slide)

So we can write: $\sigma_z^2 = \mathbf{u}_1^T \lambda \mathbf{u}_1 = \lambda \mathbf{u}_1^T \mathbf{u}_1 = \lambda$

Variance corresponding to our first principle component

Therefore we choose as our first principle component the eigenvector that corresponds to the **largest eigenvalue**

The first PC will account for the most variance, the second PC to the second most, etc.

# PCA: Variance explained

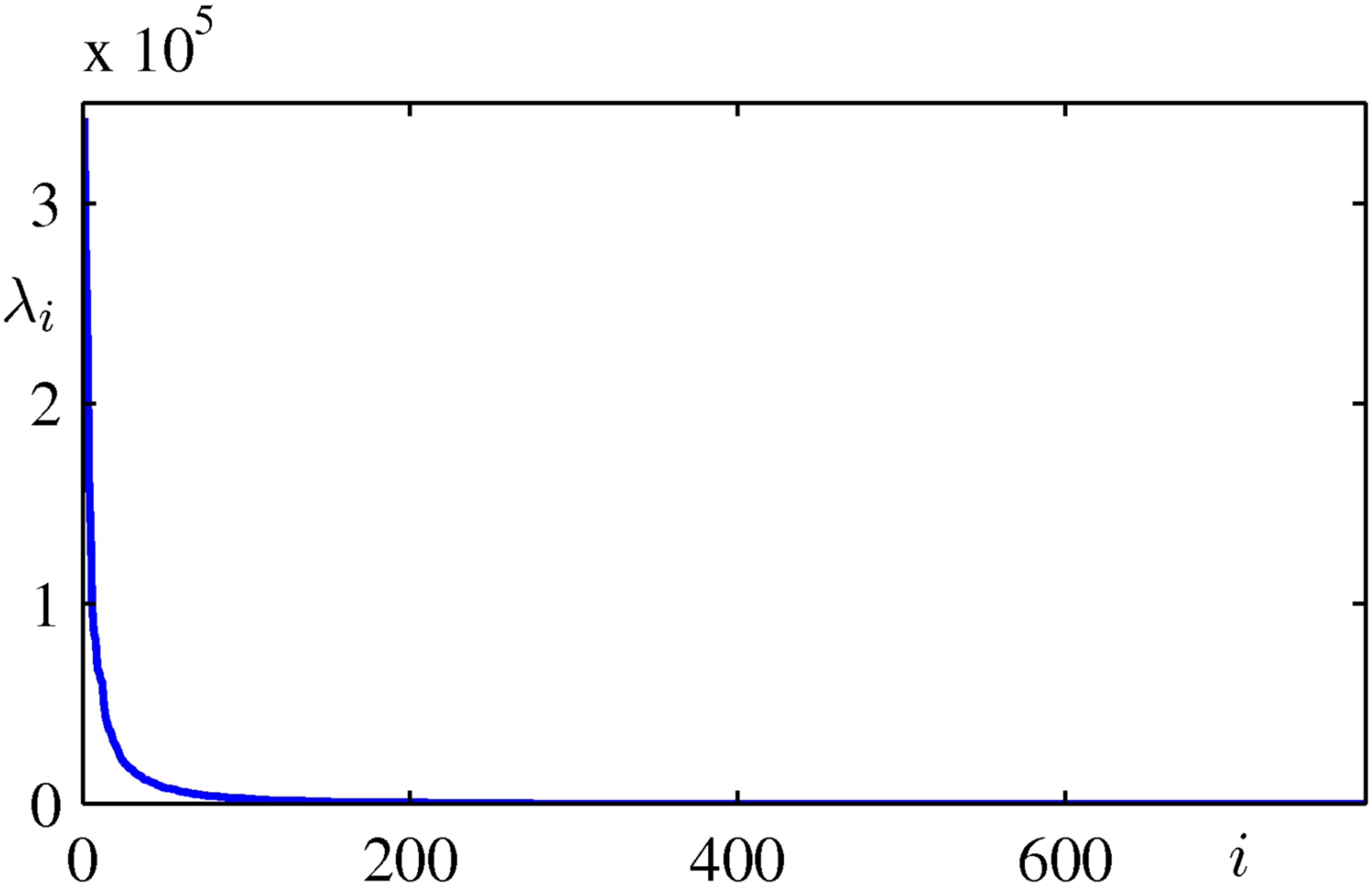
The **fraction of variance explained** $= \dfrac{\sum_{i=1}^{M} \lambda_i}{\sum_{i=1}^{D} \lambda_i}$

$M$ = dimensionality of the subspace

$D$ = dimensionality of the original data space

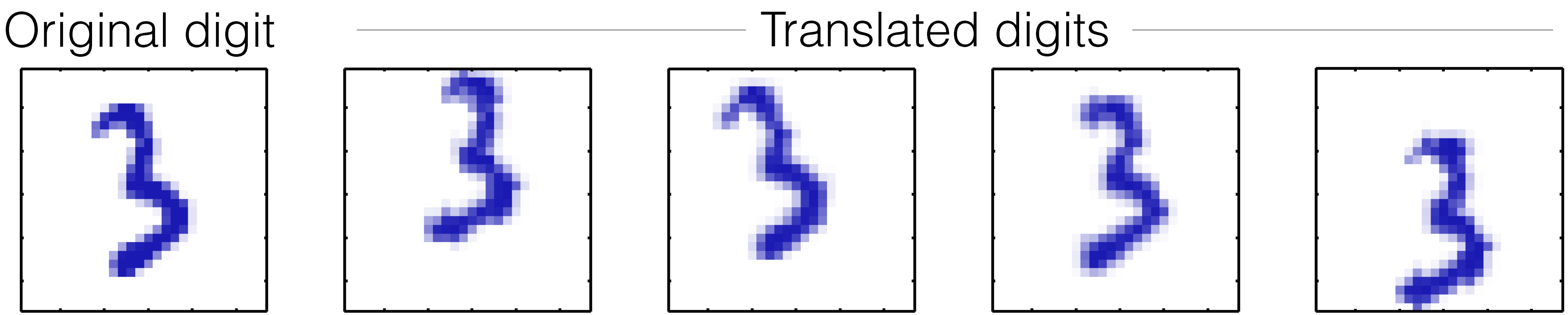
The more principle components included, the more of the variance will be represented in the projected data

# Eigenvalues by principal component $i$




Bishop, Pattern Recognition, 2006

# Example: translated digits




**Types of translation**:
1. Horizontal translation
2. Vertical translation
3. Rotation

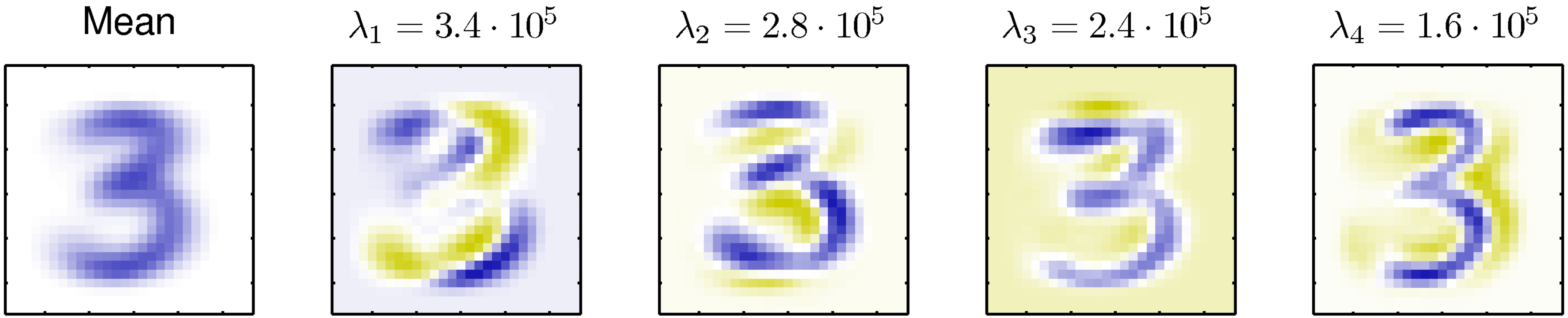
Original digits: 64 x 64 pixels

New size: 100 x 100 pixels

Bishop, Pattern Recognition, 2006

# Example: translated digits

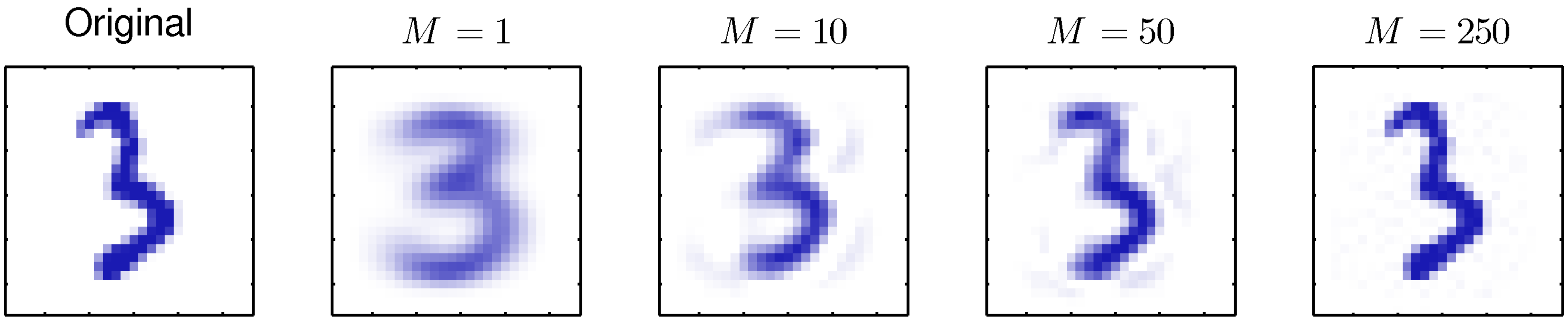
Examples of first four principle component eigenvectors and eigenvalues:




Bishop, Pattern Recognition, 2006

# Example: translated digits

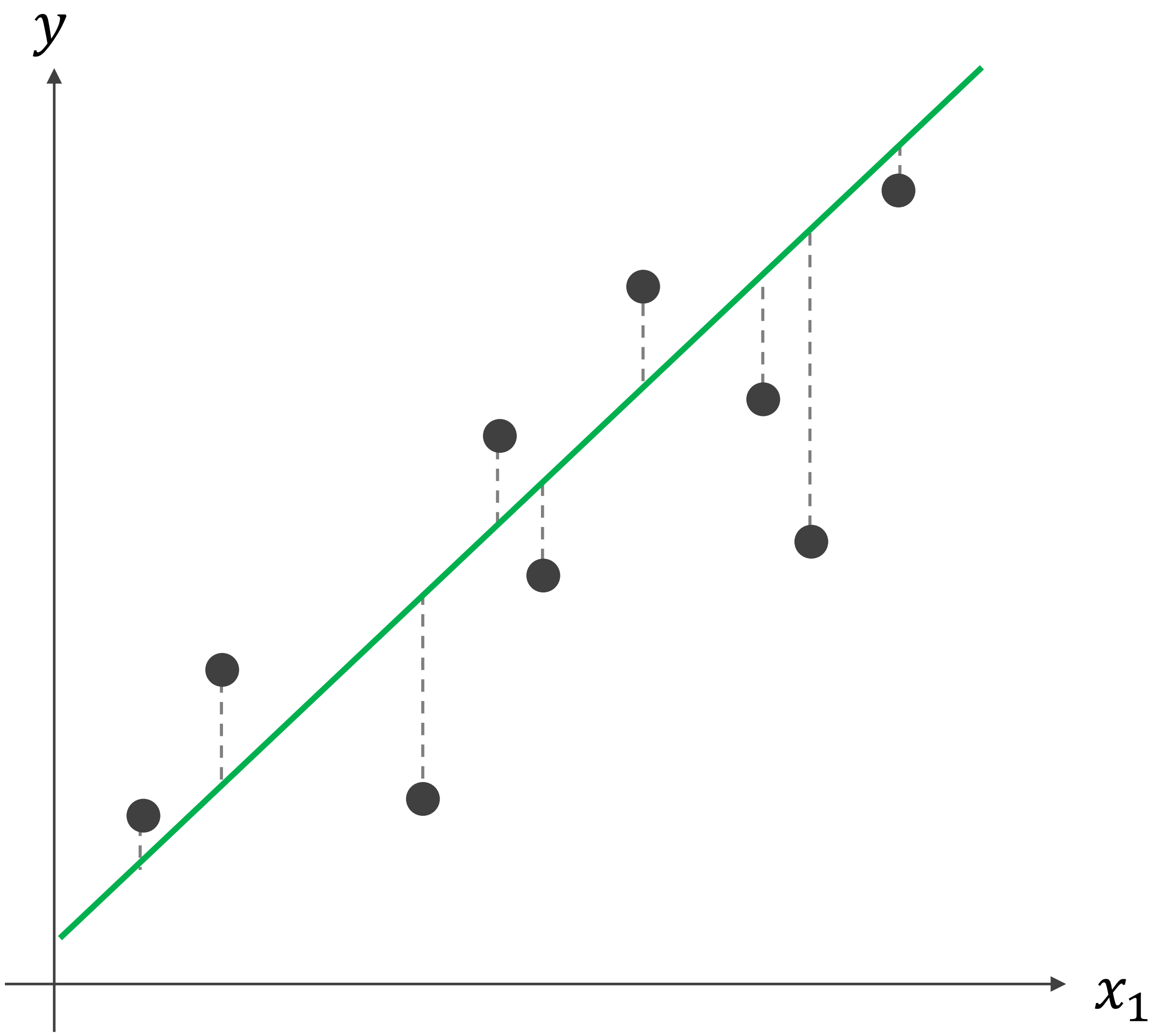
Reconstructed examples using different numbers of principal components:



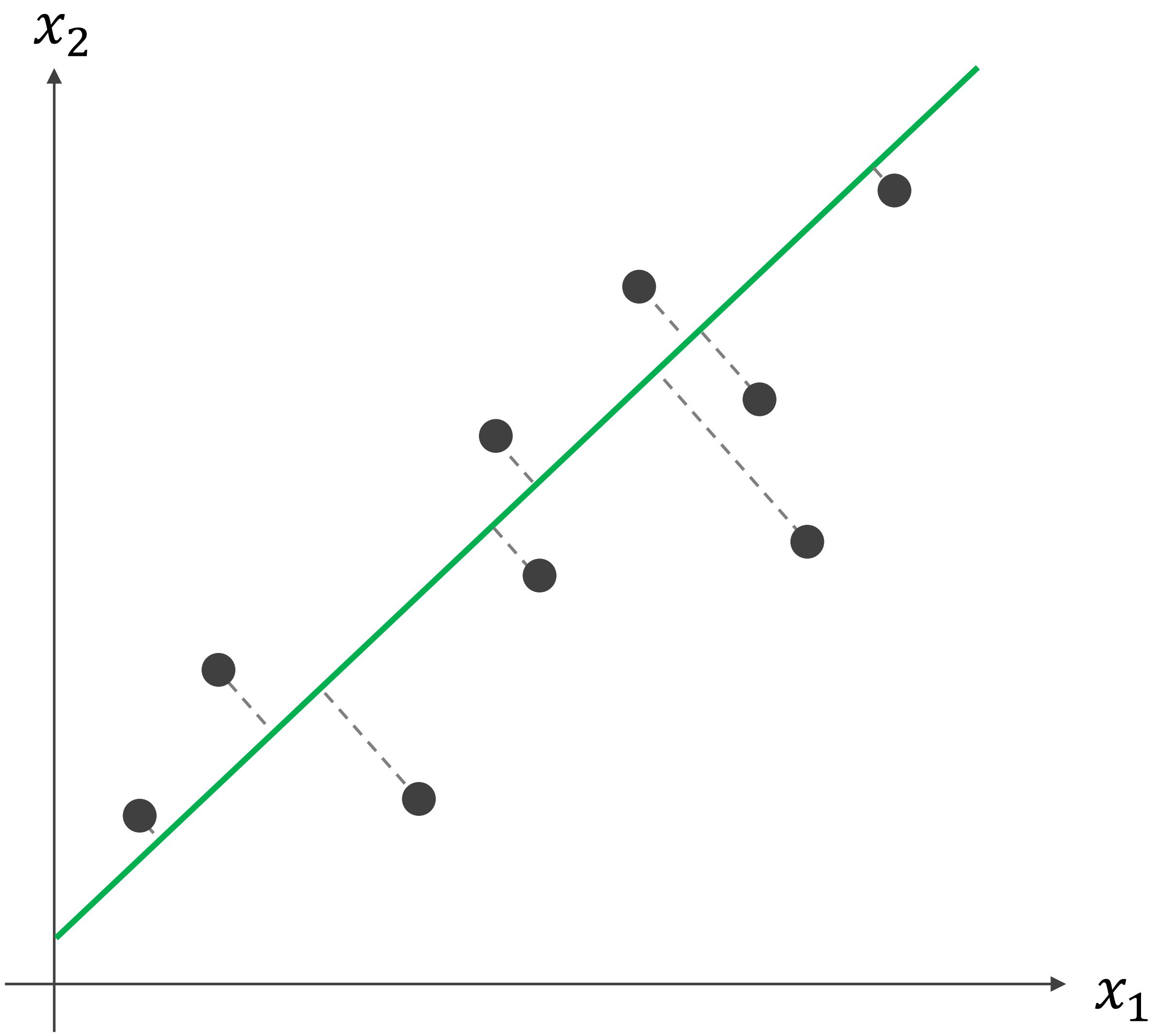

Bishop, Pattern Recognition, 2006

# Relationship between the objective for least squares and PCA

Linear regression




First principal component



# Extracting principal components

size | example

**0** **Goal**: reduce the dimensionality of our data from $D$ to $M$, where $\mathrm{M} < D$

columns = features ($D$)

$$\mathbf{X} = \begin{bmatrix} x_{11} & \cdots & x_{1D} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{ND} \end{bmatrix}$$

rows = observations ($N$)

$[N \times D]$

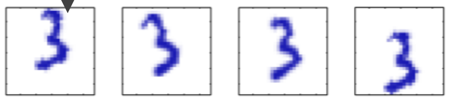
**1** Normalize each feature to mean zero and a standard deviation of 1

Each observation as a vector:

$\mathbf{x}_i \quad i = 1, \ldots, D$

$[D \times 1]$

Each pixel represents a feature



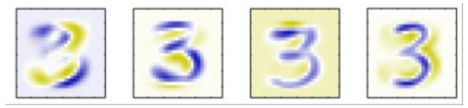
$\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \mathbf{x}_4$

**2** Determine the principal components

Calculate the eigenvectors and eigenvalues of the data covariance matrix, $\boldsymbol{\Sigma}$

Eigenvectors in descending order of their eigenvalues are the principal components

$\mathbf{u}_i$ eigenvectors / principal components $[D \times 1]$



$\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3 \quad \mathbf{u}_4$

$\lambda_i$ eigenvalues (how much of the variance is explained) [scalar]

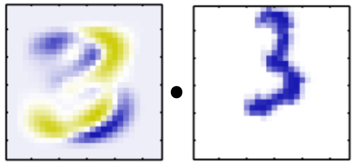
$i = 1, \ldots, D$

**3** Project the data features on the principal components

$$z_{ij} = \mathbf{u}_j^T \mathbf{x}_i \qquad j = 1, \ldots, D \quad i = 1, \ldots, N$$

[scalar]

$\mathbf{u}_1 \cdot \mathbf{x}_1 = z_{11}$



$= 2.43$

$[D \times 1] \quad [D \times 1] [\text{scalar}]$

**4** Keep the top $M$ principal components to reduce into a lower dimension

$$\mathbf{A} = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_M] \qquad [D \times M]$$

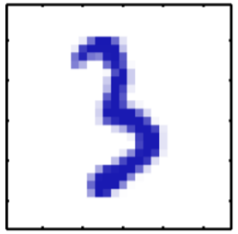
$$\mathbf{z}_i = \mathbf{A}^T \mathbf{x}_i \qquad i = 1, \ldots, N$$

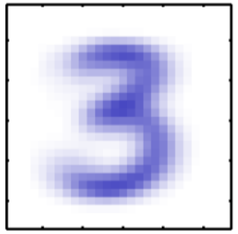
Images from Bishop, Pattern Recognition, 2006

# Reconstructing our data from principal components

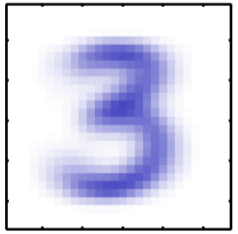
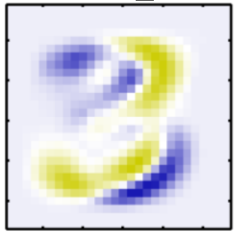
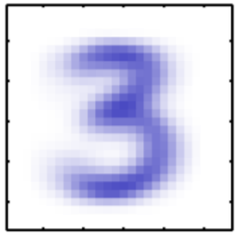
Sum the product of our projected data, $\mathbf{z}_i$, and our principle components

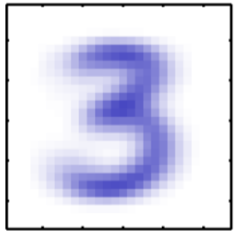
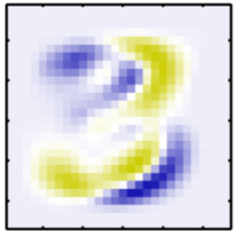
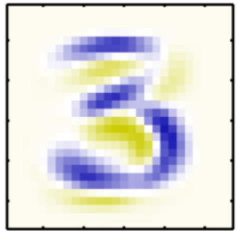
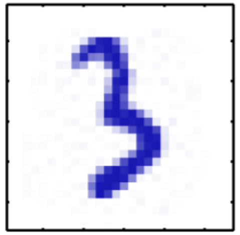
$$\hat{\mathbf{x}}_i = \sum_{j=1}^{M} z_{ij}\mathbf{u}_j$$

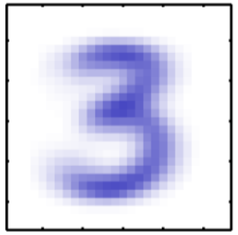
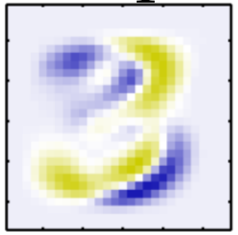
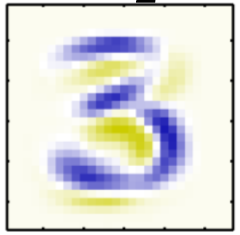
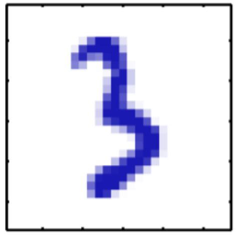
Example: the ith observation: $\mathbf{x}_i =$ 

$\bar{\mathbf{x}} =$ 

PCA-projected data: $\mathbf{z}_i = [z_{i1}, z_{i2}, \dots, z_{iM}]$

$M = 1$ $\hat{\mathbf{x}}_i =$ $\bar{\mathbf{x}}$  $+z_{i1} \cdot$ $\mathbf{u}_1$  $=$ 

$M = 250$ $\hat{\mathbf{x}}_i =$ $\bar{\mathbf{x}}$  $+z_{i1} \cdot$ $\mathbf{u}_1$  $+z_{i2} \cdot$ $\mathbf{u}_2$  $+\sum_{j=3}^{250} z_{ij}\mathbf{u}_j$ $=$ 

$M = 10{,}000$ $\hat{\mathbf{x}}_i =$ $\bar{\mathbf{x}}$  $+z_{i1} \cdot$ $\mathbf{u}_1$  $+z_{i2} \cdot$ $\mathbf{u}_2$  $+\sum_{j=3}^{10{,}000} z_{ij}\mathbf{u}_j$ $=$ 

(perfect reconstruction)

Images from Bishop, Pattern Recognition, 2006

# Why PCA?

- Dimensionality reduction
- Feature extraction
- Data visualization
- Reducing feature correlation
- Lossy data compression

# Other dimensionality reduction techniques

## e.g. Manifold Learning

- Kernel PCA
- Random projections
- Multidimensional scaling
- Locality sensitive hashing
- Autoencoders
- Isomap