Dimensionality Reduction

The **Curse** of Dimensionality

High dimensions = lots of features

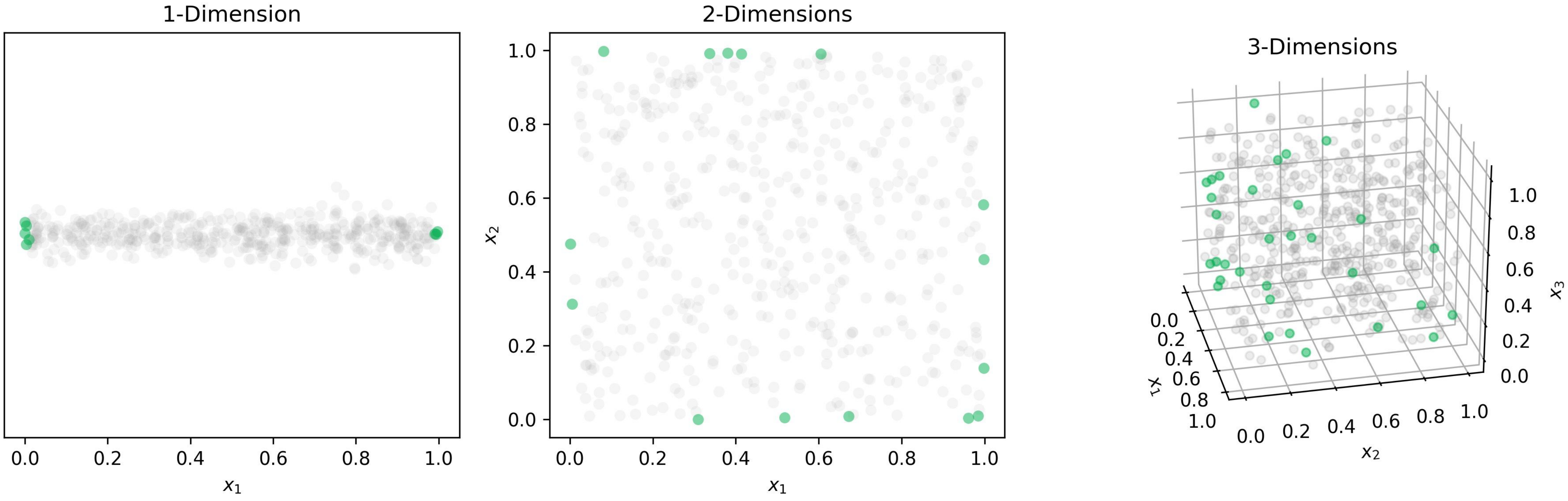
Challenge 1

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



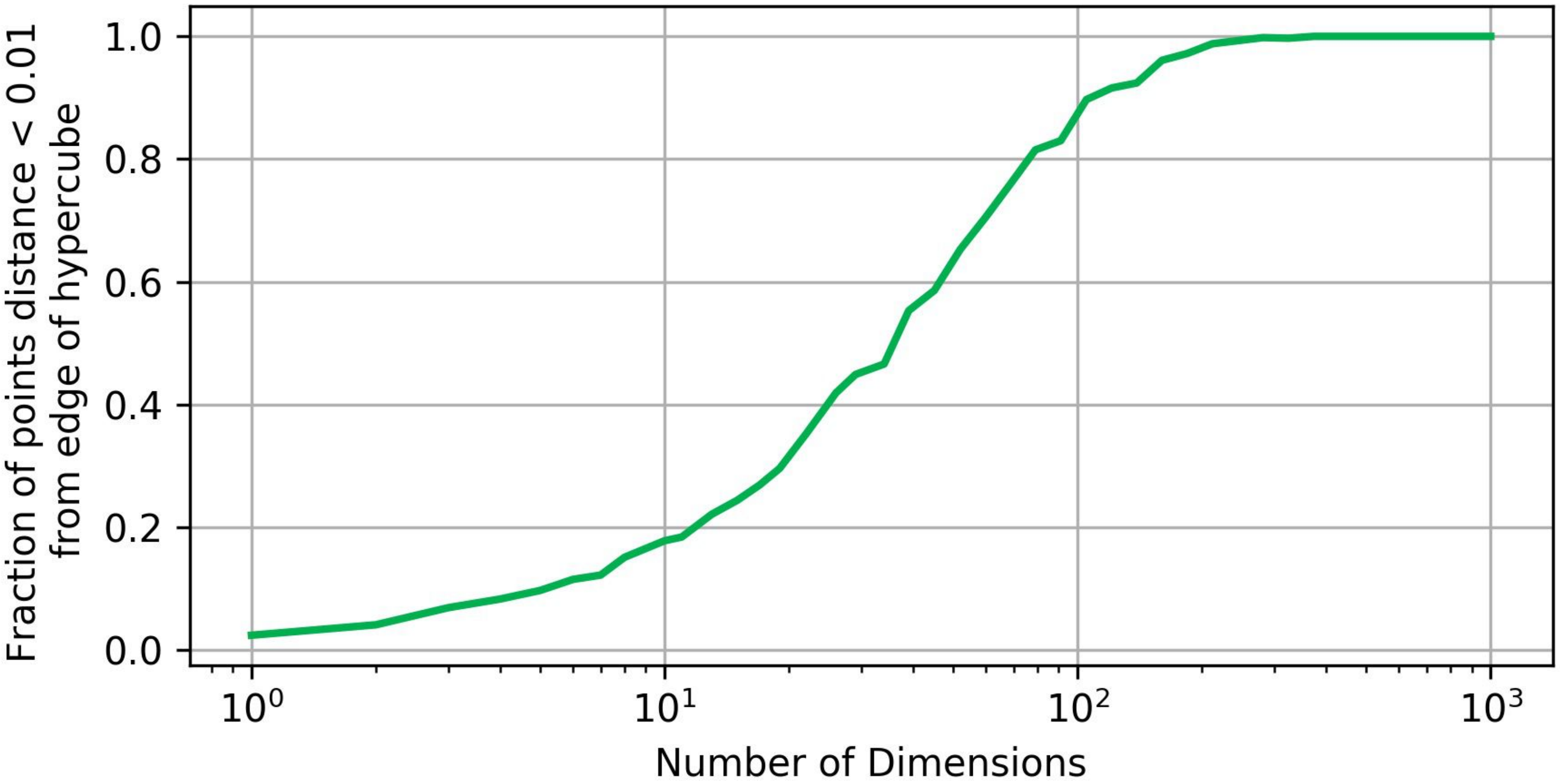
Fraction of edge data =

0.016

0.030

0.064

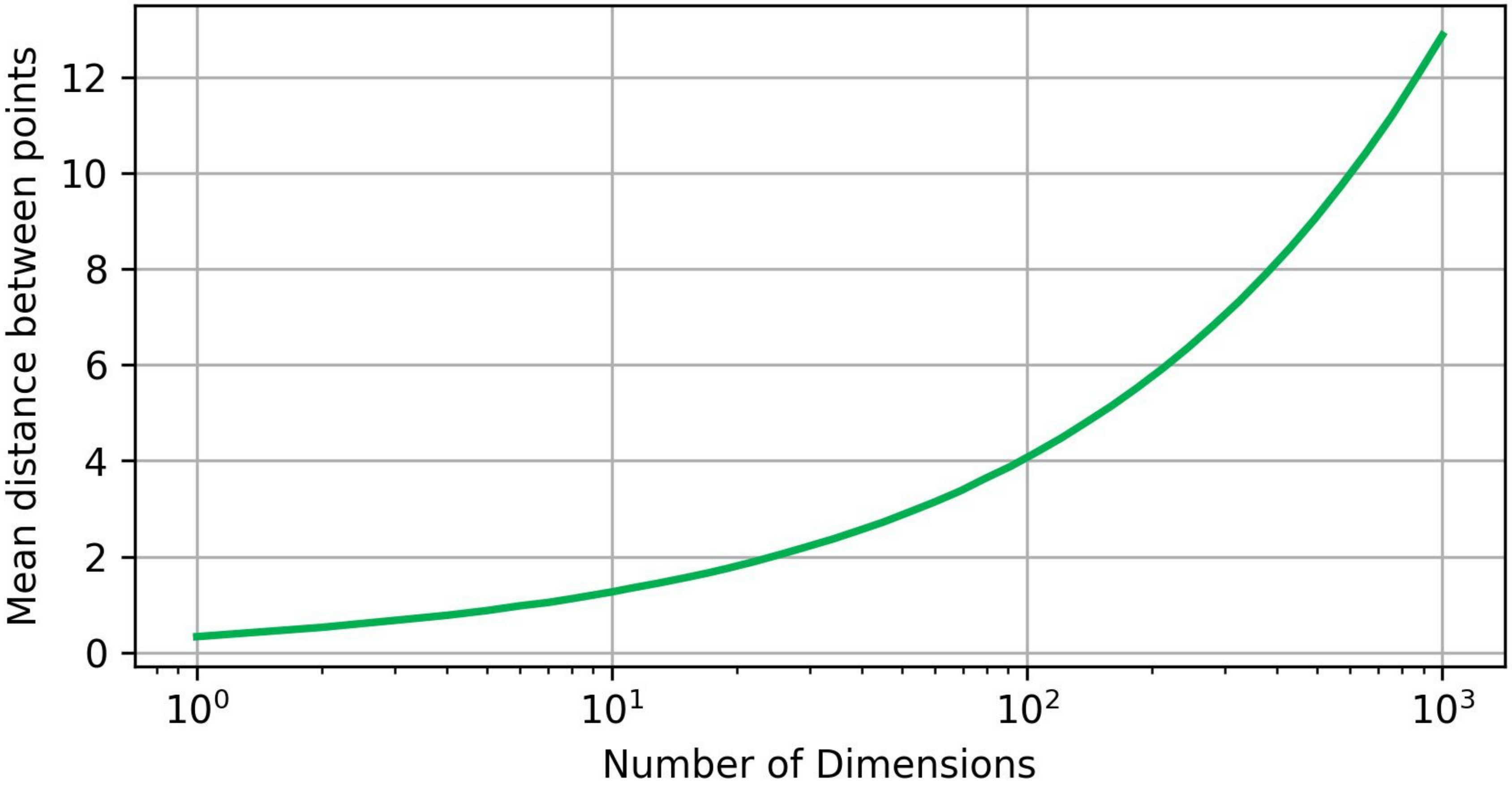
In high dimensions…



…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

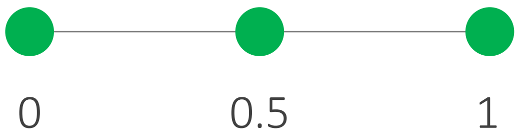
Note: figures constructed using 1,000 random points

Challenge 2

Much more data are needed for sampling higher dimensional spaces

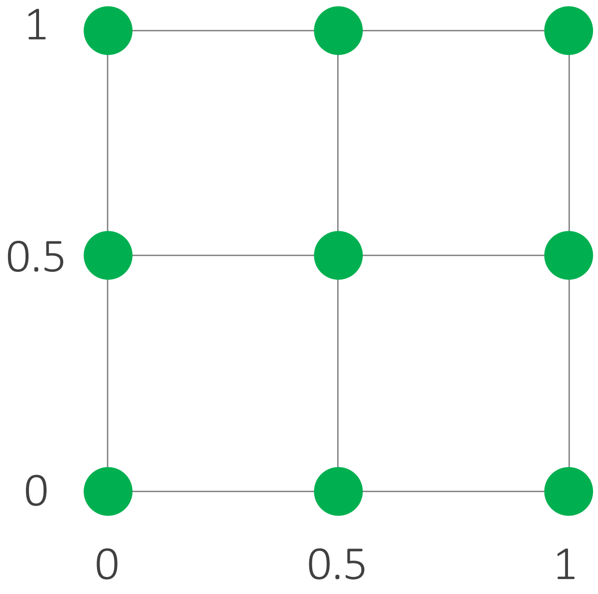
Sample a unit hypercube on a grid spaced at intervals of 0.5

D = 1



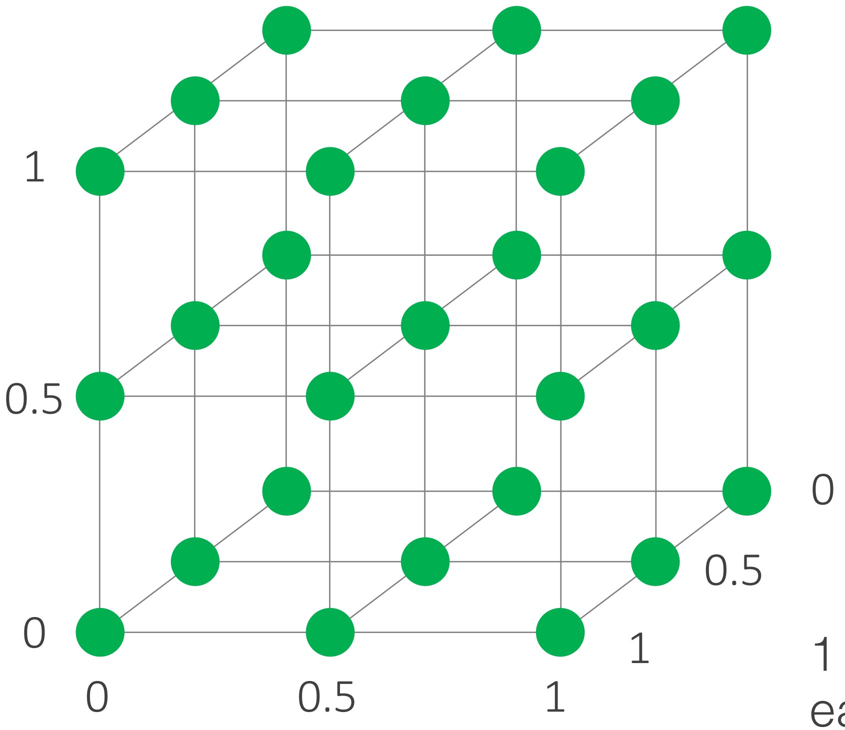
N = 3

D = 2



N = 9

D = 3



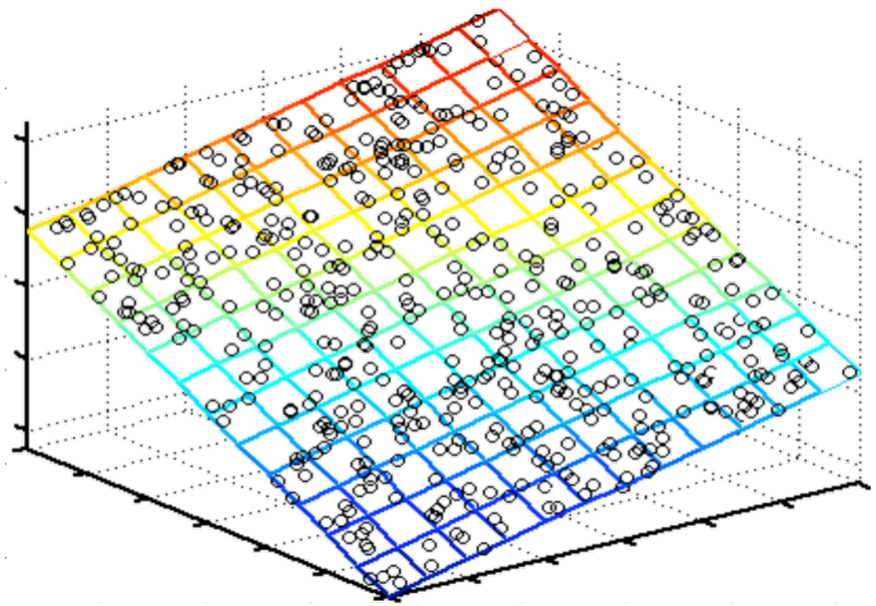
N = 27

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

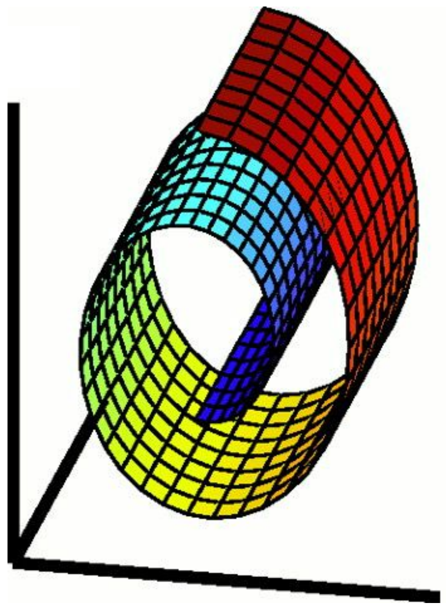
1 million Googles, each with 20 exabytes of data would only be 10^{25} bytes

…it takes more data to learn in high dimensional spaces

Data may lie in lower dimensional subspaces



Linear structure between features



Nonlinear structure between features

Often features are related to one another (are combinations of other features)

High dimensional data often exist in a lower dimensional subspace

Image Left: Torki, M. and June, Dissertation, 2011. Learning the manifolds of local features and their spatial arrangements. Rutgers University.
Image Right: Roweis, S.T. and Saul, L.K., 2000. Nonlinear dimensionality reduction by locally linear embedding. science, 290(5500), pp.2323-2326.

Our Goal:

Find a lower dimensional representation of the data while minimizing the projection error relevant to your application

Dimensionality Reduction

Benefits:

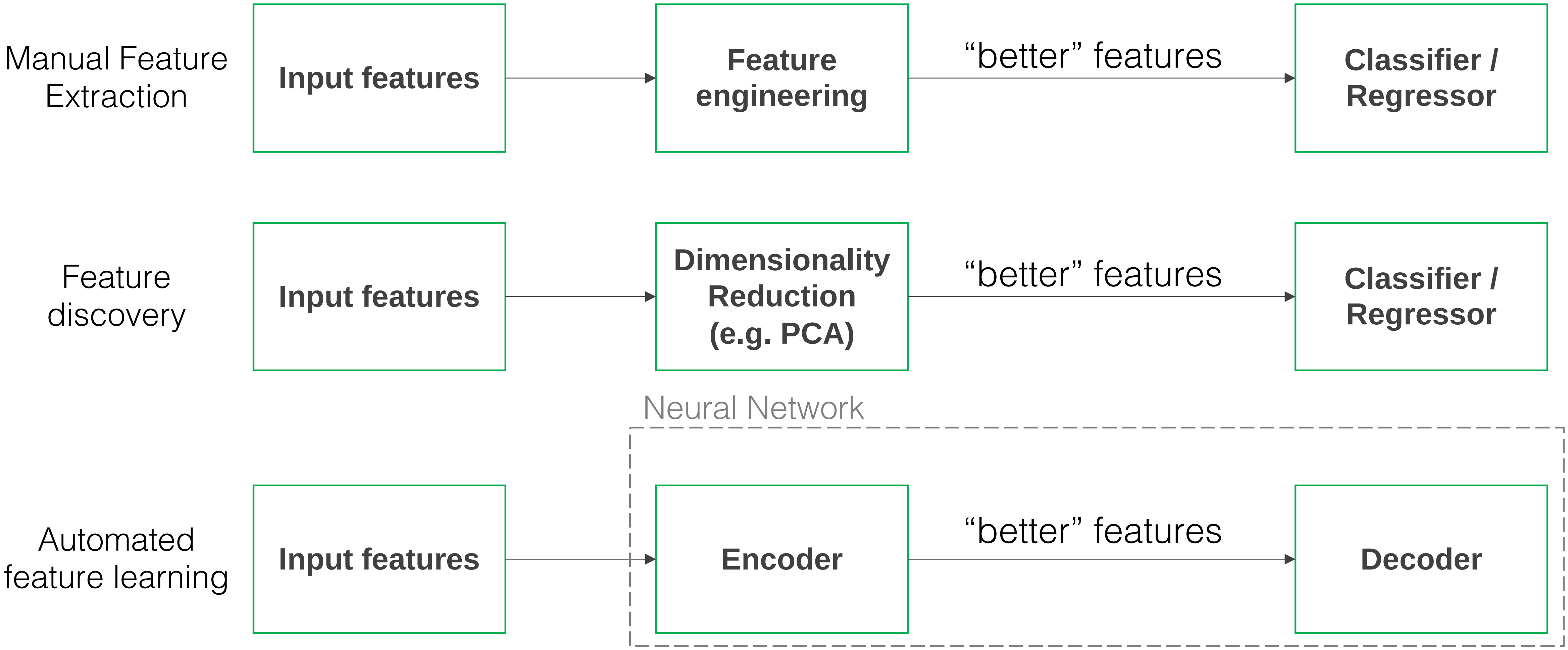
Simplified computation
Reduced redundancy of features
Improved numerical stability due to removed correlations

Common approaches:

Feature selection techniques (we discussed previously)
Principal Components Analysis (PCA)
Linear Discriminant Analysis (LDA) [supervised]
Non-negative Matrix Factorization (NMF)
Multidimensional scaling (MDS)
Autoencoder
t-distributed Stochastic Neighbor Embedding (t-SNE)
Uniform Manifold Approximation and Projection (UMAP)

Feature projection techniques

Another perspective:
Representation Learning



PCA

Before you begin: Normalize the data!

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

Normalized feature

Raw, unscaled feature

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

columns = features

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

rows = observations

We normalize each of the columns
N = number of samples
D = number of features

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

$$\mathbf{A} \quad \mathbf{x} \quad \rightarrow \quad \mathbf{z}$$

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

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

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

PCA Features are linear combinations of the input features

$$z_1 = u_{11}x_1 + u_{12}x_2 + \cdots + u_{1D}x_D$$

$$z_2 = u_{21}x_1 + u_{22}x_2 + \cdots + u_{2D}x_D$$

$$\vdots$$

$$z_M = u_{M1}x_1 + u_{M2}x_2 + \cdots + u_{MD}x_D$$

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 in $\mathbb{R}^D$

The i^{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

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

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

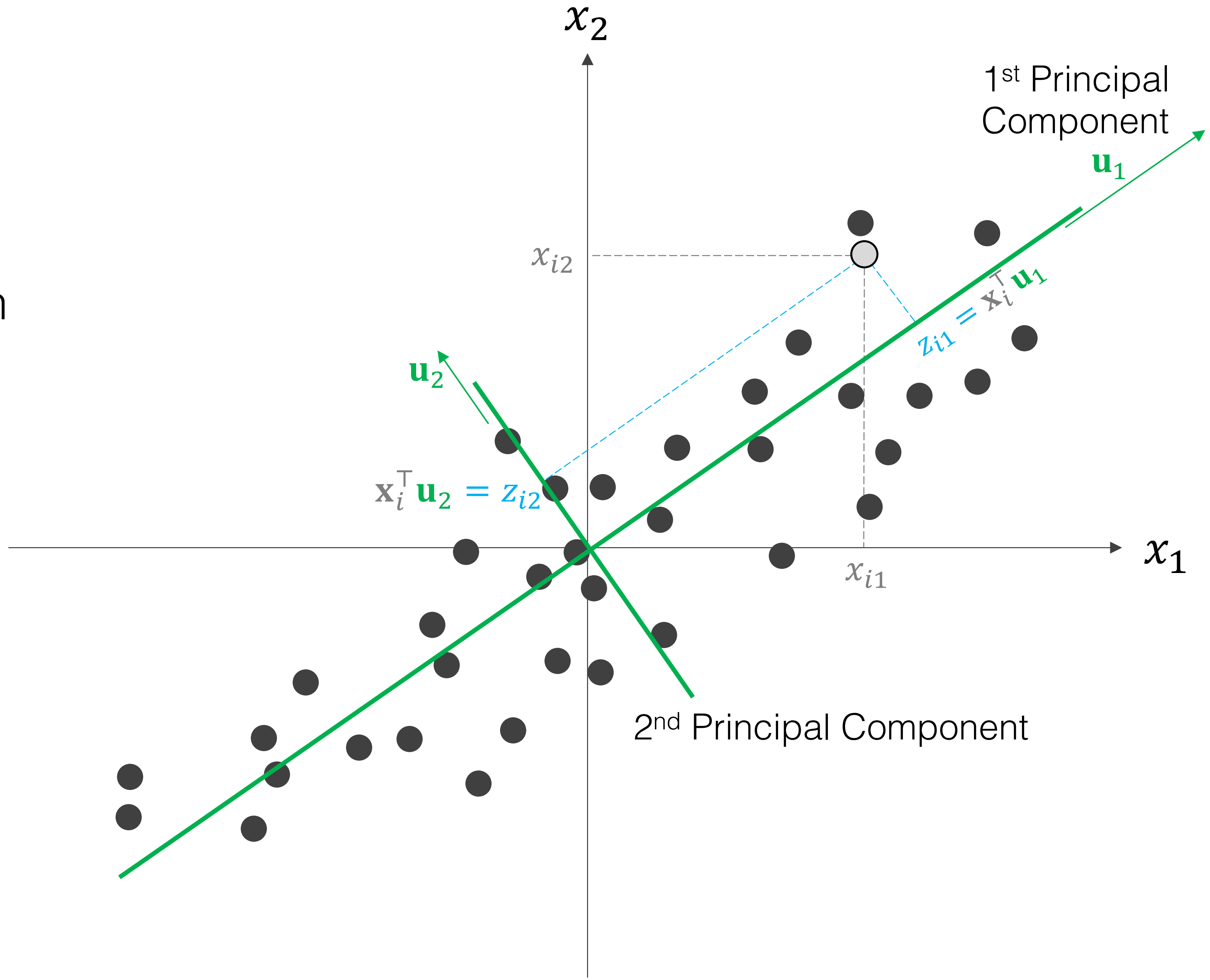
We seek to project each point $\mathbf{x}_i$ onto a unit PC vector. $z_i = \mathbf{u}_1^T \mathbf{x}_i$

Principal Components

Maximum variance formulation

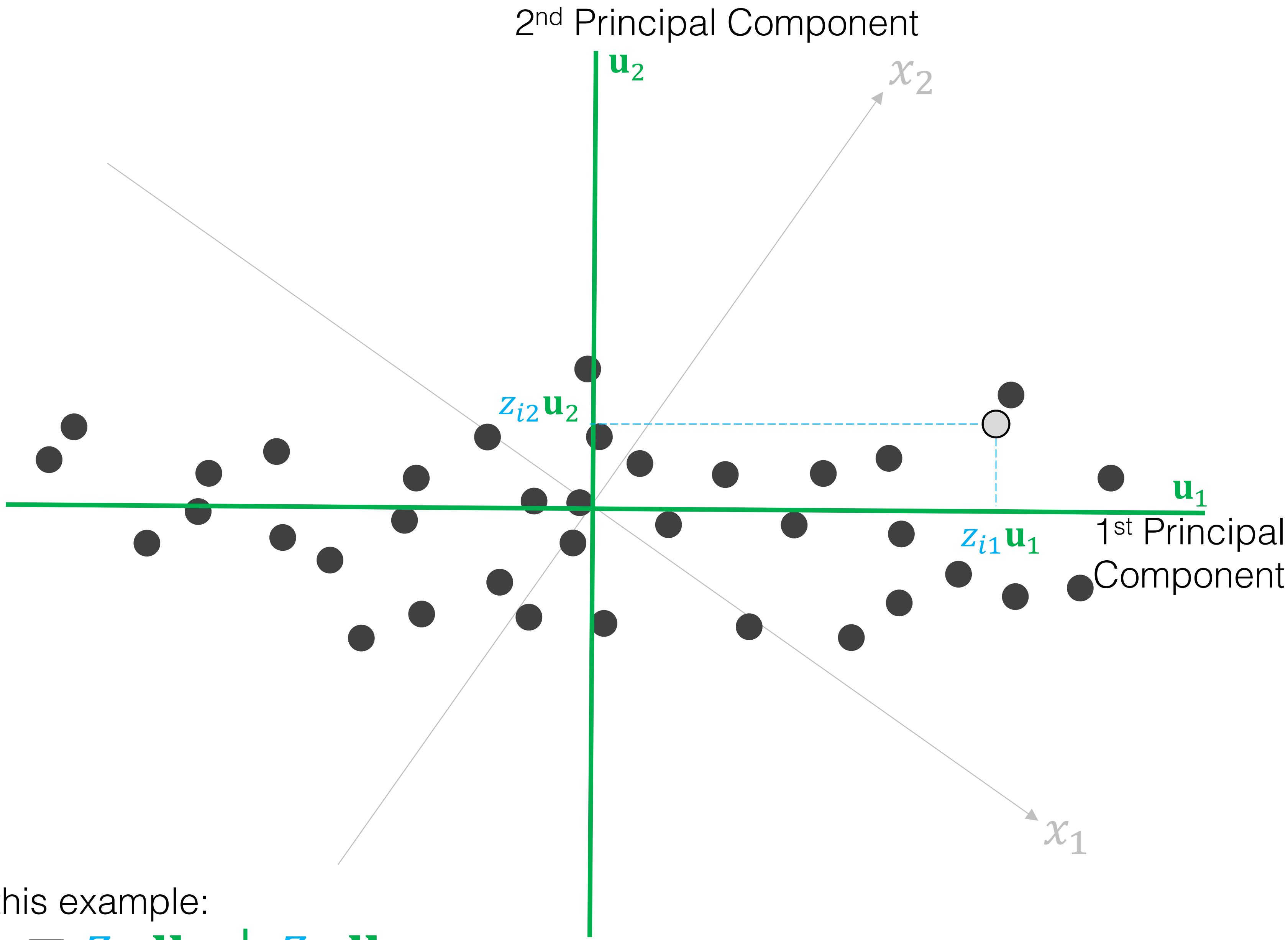
Length of a projection
onto a unit vector:

$$z_{i1} = \mathbf{x}_i^\top \mathbf{u}_1$$



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

Reprojected Data onto Principal Components



Any point $\boldsymbol{x}_i$ can be represented as a combination of the principal 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 $\mathbb{R}^D$

In this example:

$$\mathbf{x}_i = z_{i1}\mathbf{u}_1 + z_{i2}\mathbf{u}_2$$

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 (projected) variance of the data 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 length on 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 variance as:

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

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

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

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 (i), Predictor index (j)

Predictors →

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

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

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

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

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

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

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

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

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

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

Mean of each predictor

If $\bar{x}_j = 0$ for all j

This will be the case IF the data are standardized

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

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

$$= E[X_j X_k]$$

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

Covariance and Correlation

Relationship between covariance and correlation

$$\text{corr}(X,Y) = \frac{\text{cov}(X,Y)}{\sqrt{\text{var}(X)\text{var}(Y)}}$$

When $\text{var}(X) = \text{var}(Y) = 1$, then:

$$\text{corr}(X,Y) = \text{cov}(X,Y)$$

If each of the features have been standardized, this means this matrix is:

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

Covariance matrix properties

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

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

All eigenvalues are non-negative

Eigenvectors are orthogonal

If the features (predictors), $x_1, x_2, \dots, x_D$ are independent, $\mathbf{\Sigma}$ is diagonal because $\mathbf{cov}(X_j, X_k) = 0$ 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 λ 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:

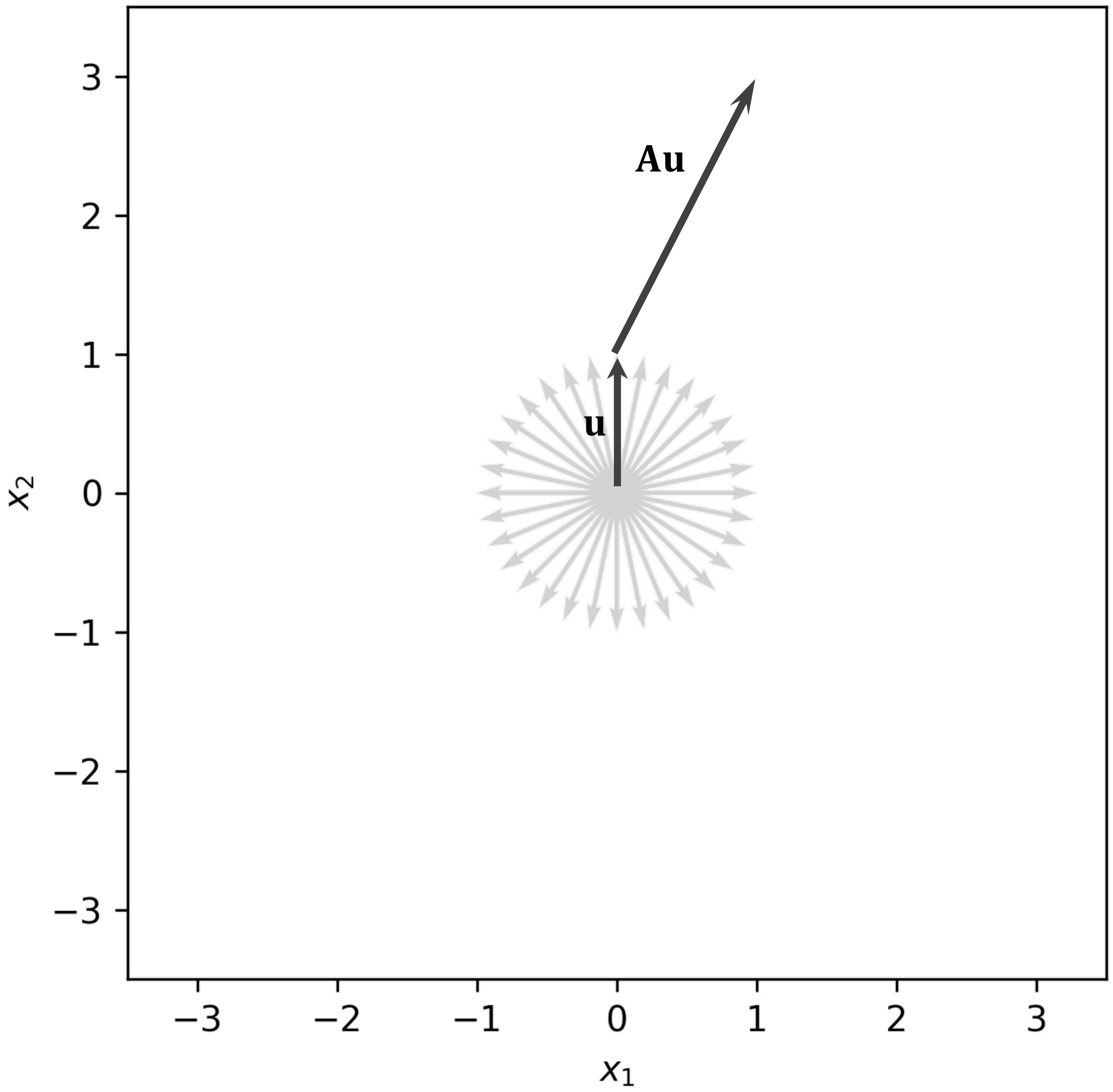
http://setosa.io/ev/principal-component-analysis/

Eigenvalues/Eigenvectors

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

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

$$\mathbf{u} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbf{Au} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

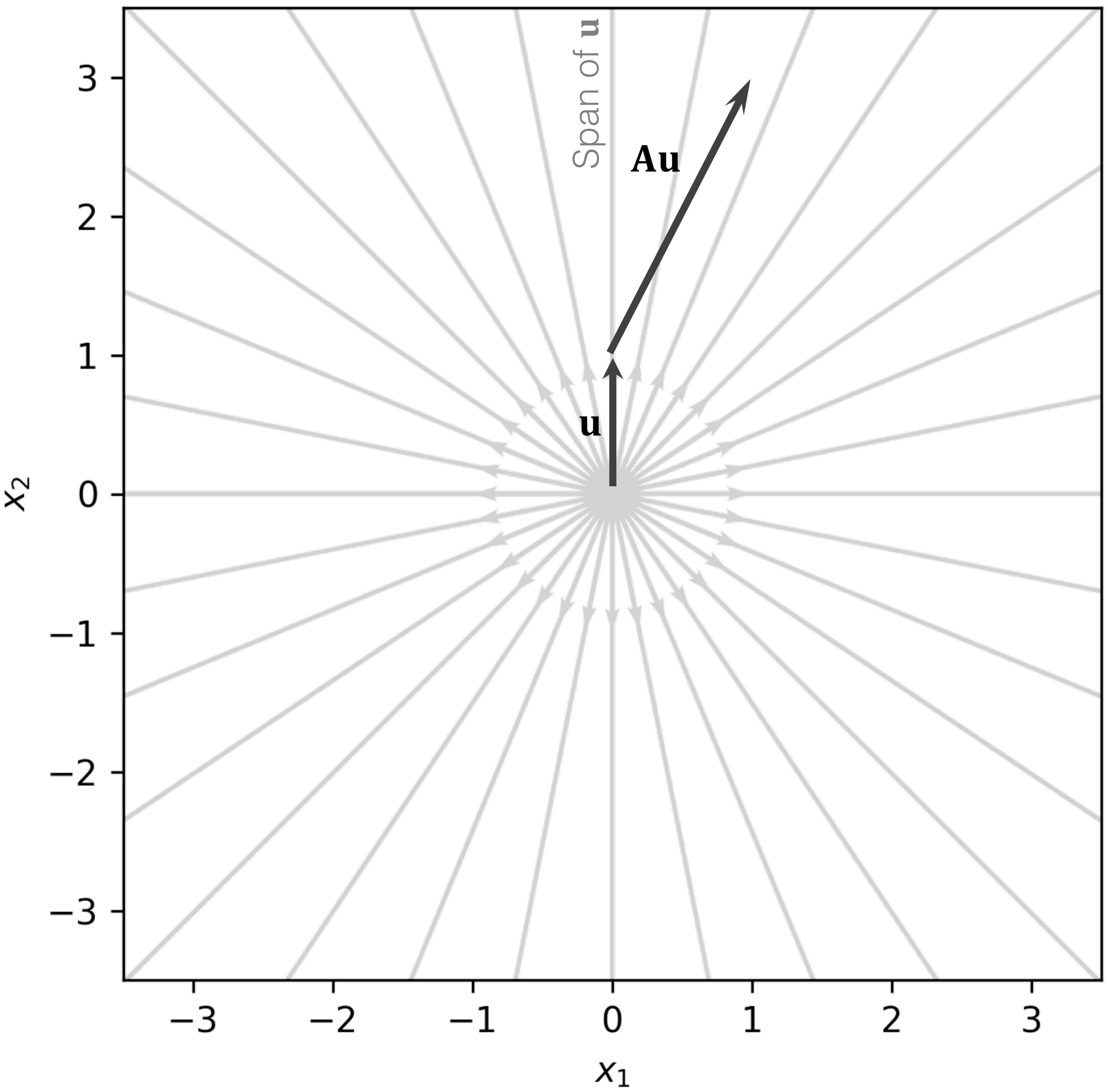


Eigenvalues/Eigenvectors

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

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

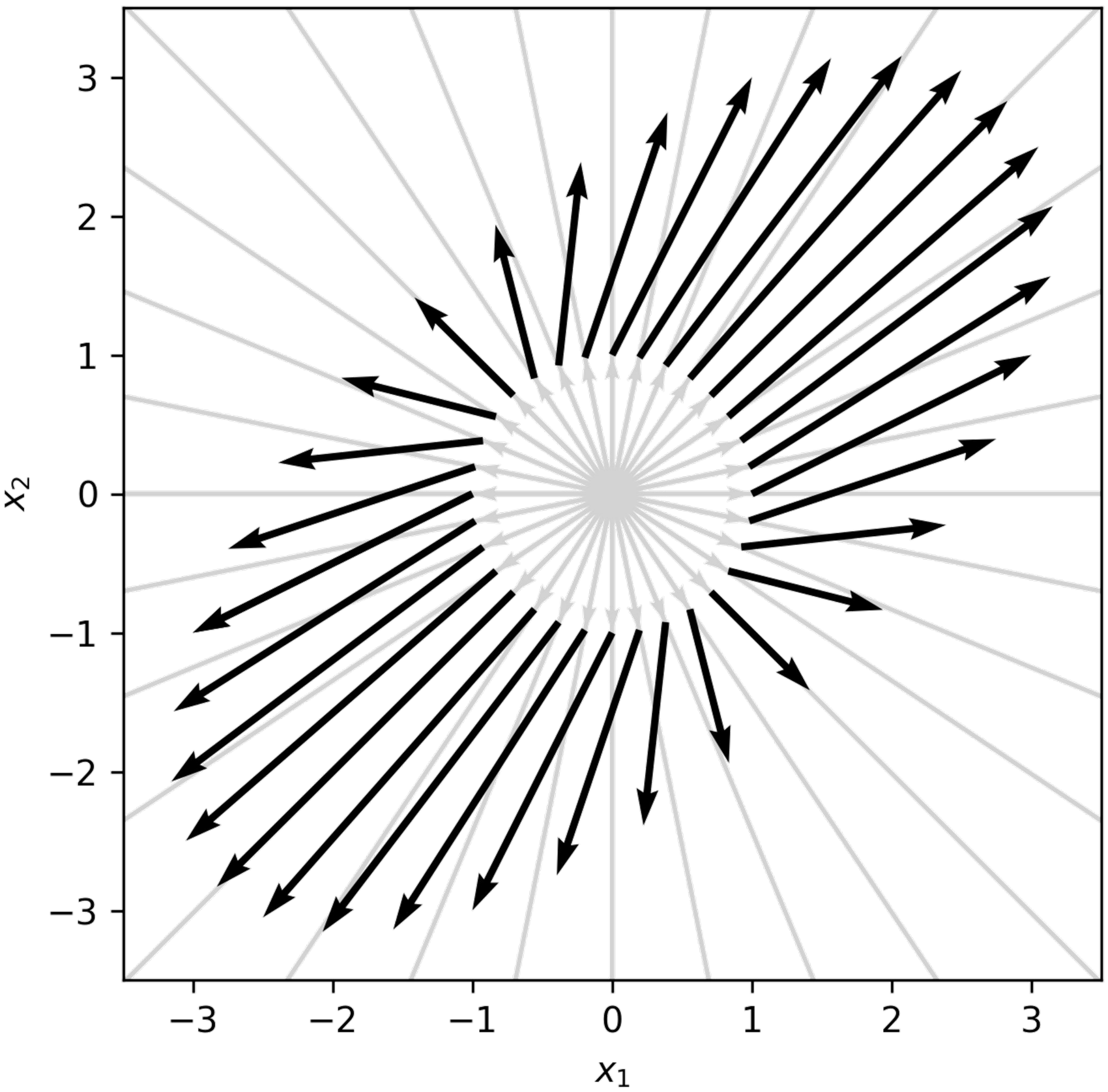
$$\mathbf{u} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbf{A}\mathbf{u} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$



Eigenvalues/Eigenvectors

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

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



Eigenvalues/Eigenvectors

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

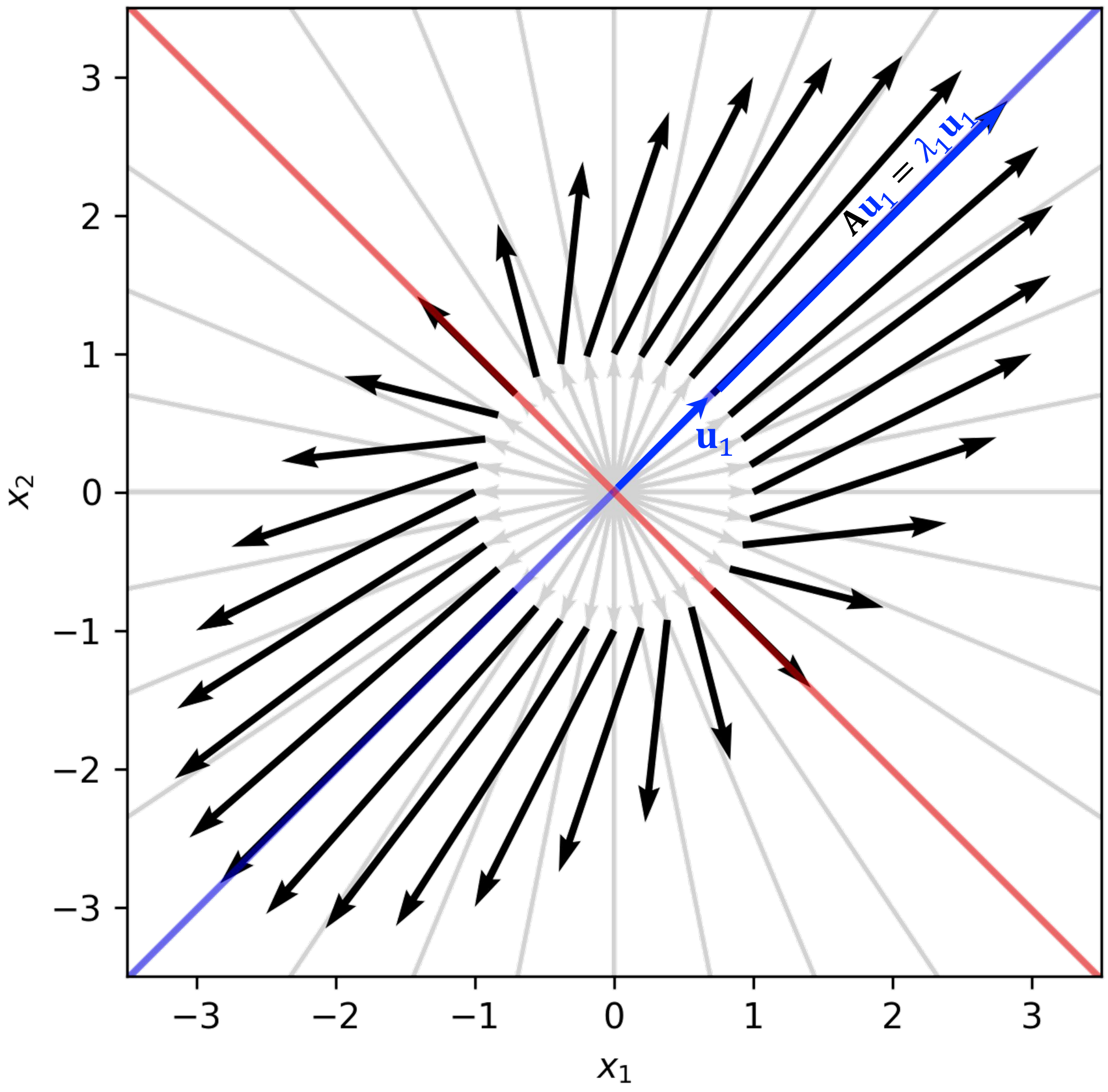
$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

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

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

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

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



PCA

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

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

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

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

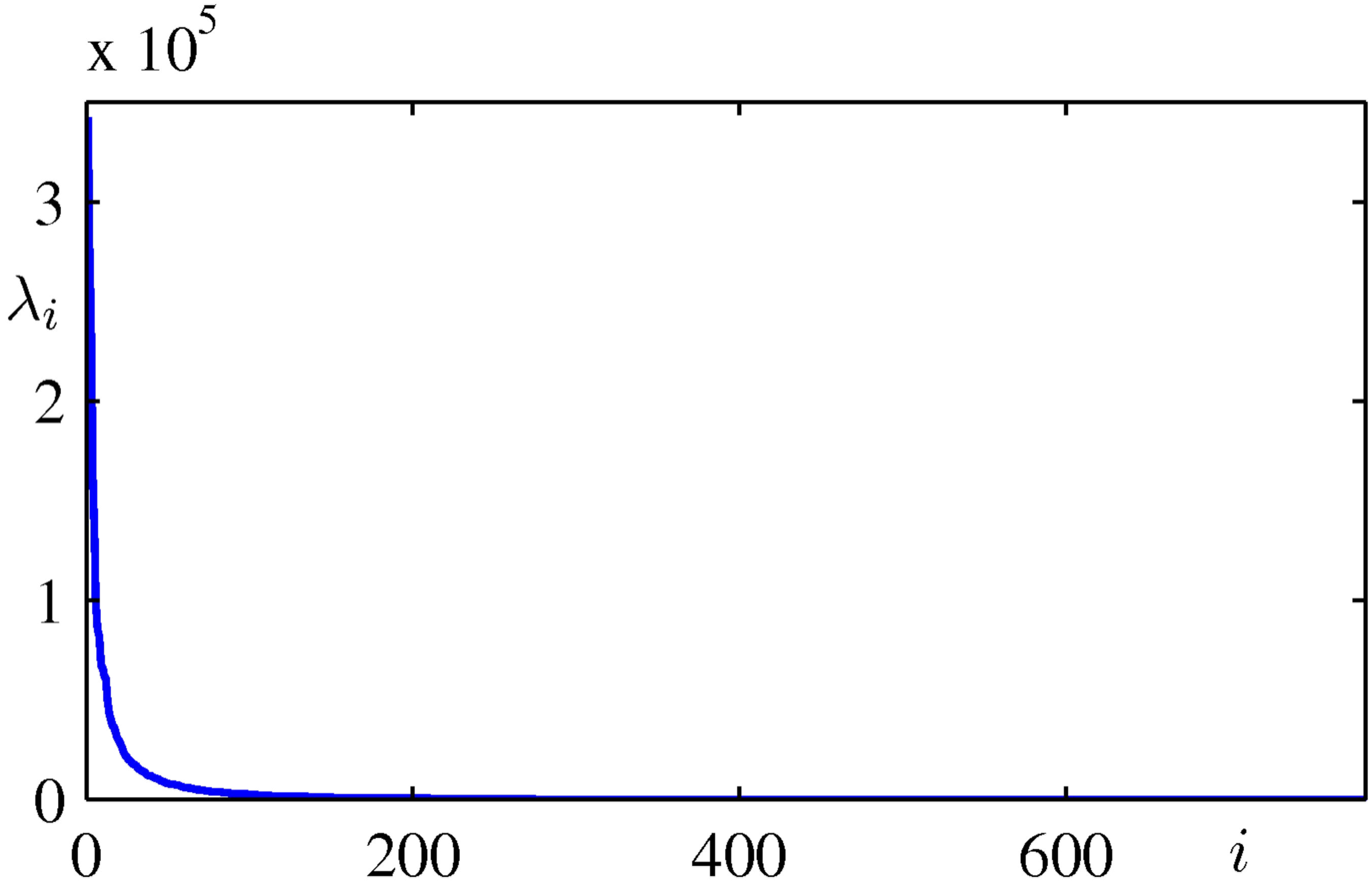
The **fraction of variance explained** $= \dfrac{\sum_{i=1}^{M} \lambda_i}{\sum_{i=1}^{D} \lambda_i}$

M = dimensionality of the subspace

D = dimensionality of the original data space

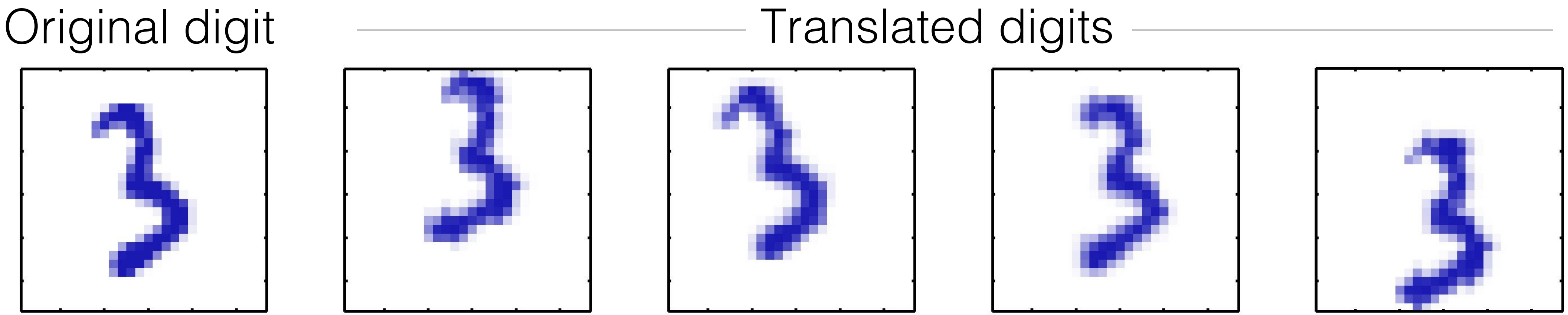
The more principle components included, the more of the variance will be represented in the projected data

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

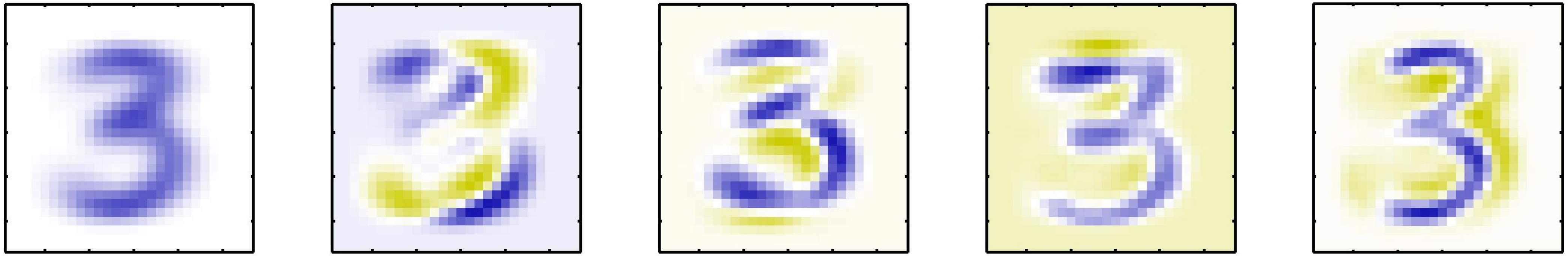
New size: 100 x 100 pixels

Bishop, Pattern Recognition, 2006

Example: translated digits

Examples of first four principle component eigenvectors and eigenvalues:

Mean $\quad \lambda_1 = 3.4 \cdot 10^5 \quad \lambda_2 = 2.8 \cdot 10^5 \quad \lambda_3 = 2.4 \cdot 10^5 \quad \lambda_4 = 1.6 \cdot 10^5$



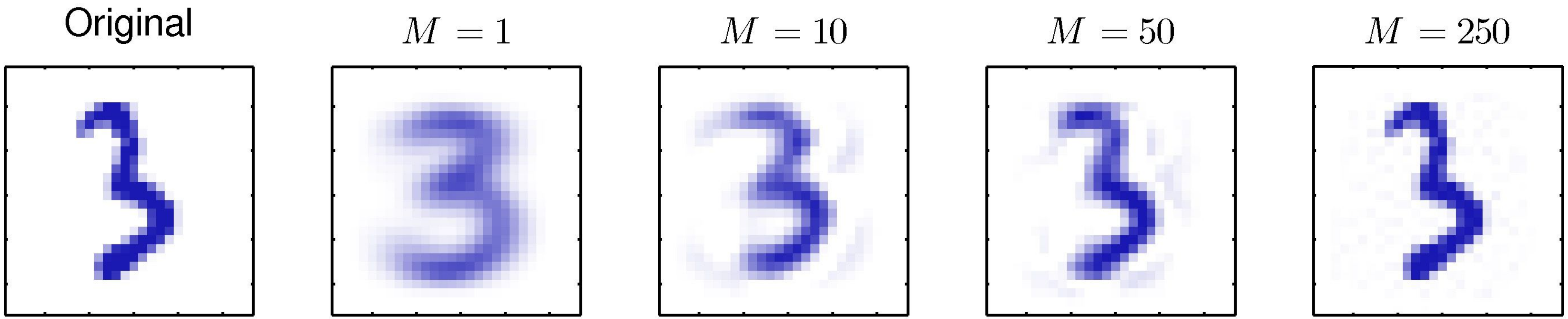
Latent Space DEMO

This links to the lower dimensional representation space of the data
(a.k.a. the latent space or embedding space) for PCA-reduced features with MNIST data

Bishop, Pattern Recognition, 2006

Example: translated digits

Reconstructed examples using different numbers of principal components:



Bishop, Pattern Recognition, 2006

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)

$[N \times D]$

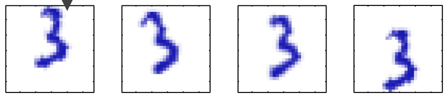
1 Normalize each feature to mean zero and a standard deviation of 1

Each observation as a vector:

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

$[D \times 1]$

Each pixel represents a feature



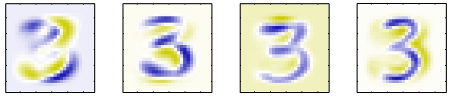
$\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \mathbf{x}_4$

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 $[D \times 1]$



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

λ_i eigenvalues (how much of the variance is explained) [scalar]

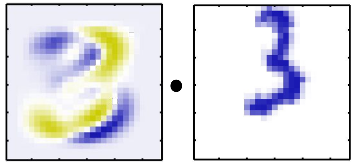
$i = 1, \dots, D$

3 Project the data features on the principal components

$$z_{ij} = \mathbf{u}_j^T \mathbf{x}_i \qquad \begin{matrix} j = 1, \dots, D \\ i = 1, \dots, N \end{matrix}$$

[scalar]

$\mathbf{u}_1 \quad \bullet \quad \mathbf{x}_1 = z_{11}$



$= 2.43$

$[D \times 1] \quad [D \times 1] \quad$ [scalar]

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

$$\mathbf{A} = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_M]$$

$[D \times M]$

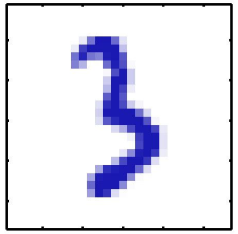
$$\mathbf{z}_i = \mathbf{A}^T \mathbf{x}_i \qquad i = 1, \dots, N$$

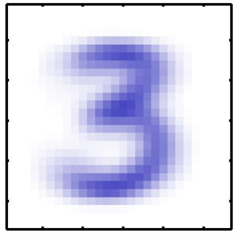
Images from Bishop, Pattern Recognition, 2006

Reconstructing our data from principal components

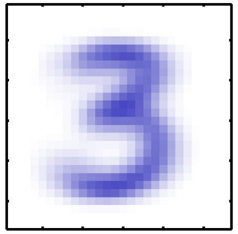
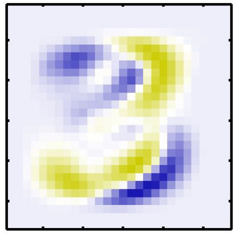
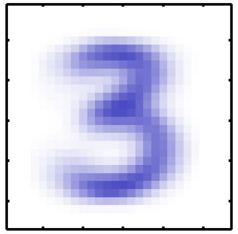
Sum the product of our projected data, $\mathbf{z}_i$, and our principle components

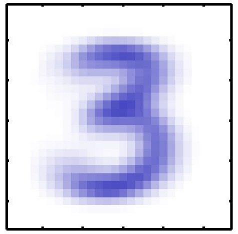
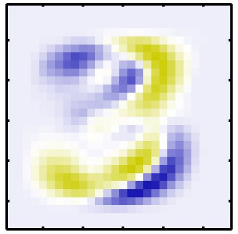
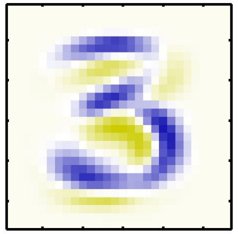
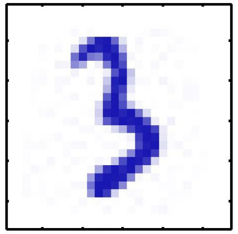
$$\hat{\mathbf{x}}_i = \sum_{j=1}^{M} z_{ij}\mathbf{u}_j$$

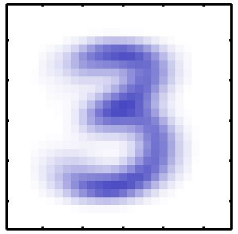
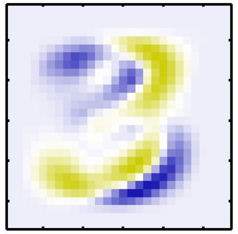
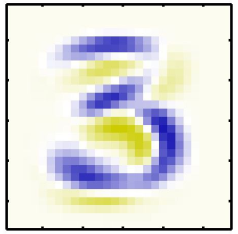
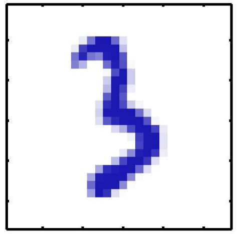
Example: the i[th] observation: $\mathbf{x}_i =$ 

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

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

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

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

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

(perfect reconstruction)

Images from Bishop, Pattern Recognition, 2006

Why PCA?

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

Other dimensionality reduction techniques

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

e.g. Manifold Learning