Day 4: Unsupervised Learning

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Learning Outcomes

By the end of this session, you will be able to:

- Differentiate between Supervised and Unsupervised Learning paradigms.
- Understand K-Means clustering, and how it could be applied to discover hidden groups in data.
- Analyze high-dimensional data using PCA and t-SNE for visualization and compression.
- Understand how Autoencoders utilize neural networks for tasks like denoising, generation, and anomaly detection.

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What is Unsupervised Learning?

So far: We've been doing **Supervised Learning**, learning from labeled data (x, y).

Supervised Learning

Data: (x, y) pairs
- x: input (features)
- y: label (target)

Goal: Learn $f(x) \approx y$

Examples:
- Image classification
- House price prediction

Unsupervised Learning

Data: Only x (no labels!)
- Just raw data
- No target to predict

Goal: Find hidden patterns or structure

Examples:
- Customer segmentation
- Data compression

Key difference: No labels $\rightarrow$ algorithm must discover structure on its own!

Why Unsupervised Learning?

Labels are expensive!

- Labeling data requires human effort, time, and expertise
- Most real-world data is unlabeled
- Sometimes we don't even know what labels to look for

The Big Idea

Can we learn useful things from data **without** labels?
Yes! Unsupervised learning finds hidden patterns, structure, and representations.

Common Unsupervised Learning Tasks

What can we do without labels?

1. Clustering
Group similar data points together
Example: Customer segmentation, document group

2. Dimensionality Reduction
Compress high-dimensional data to lower dimensions
Example: Visualization, feature extraction

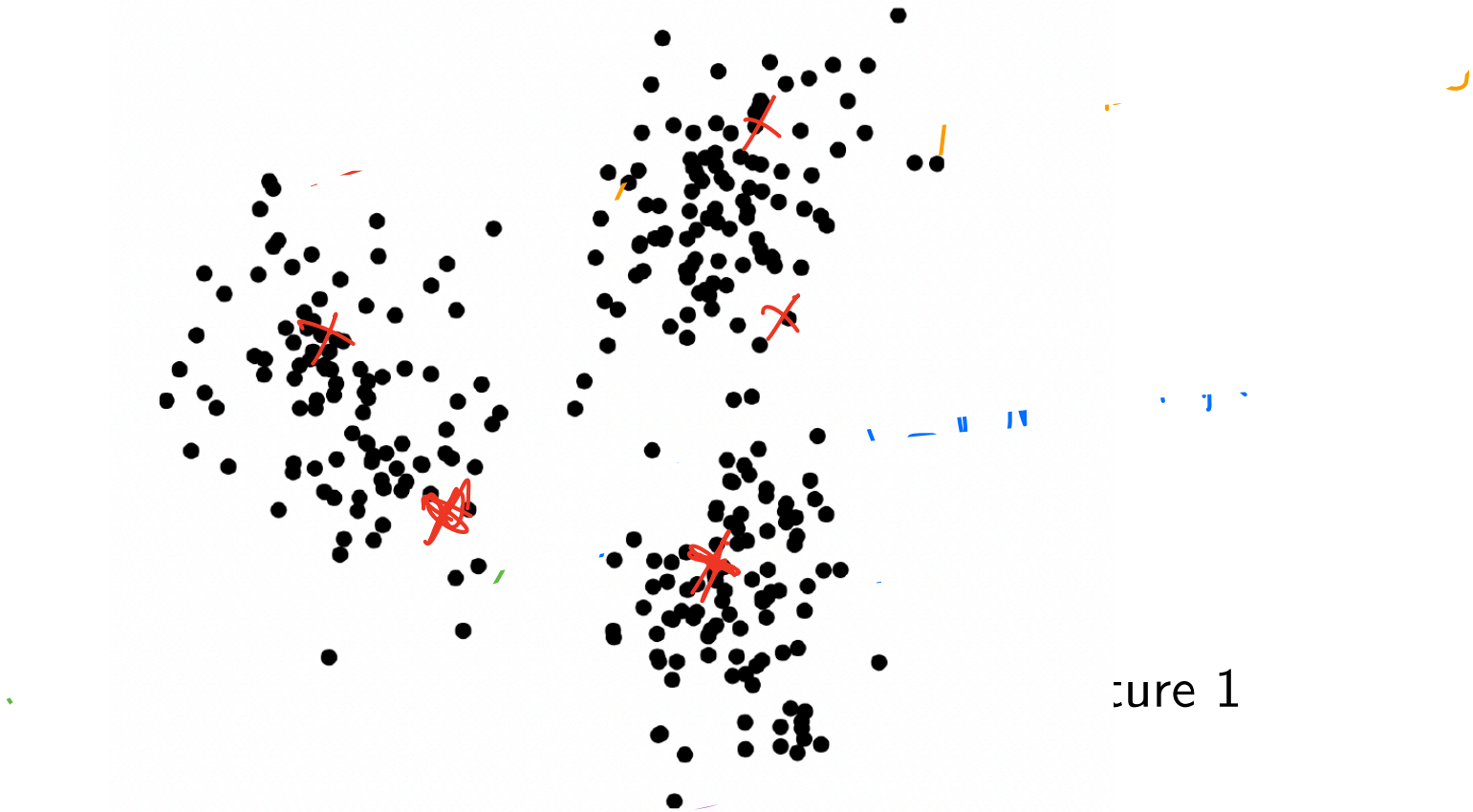
3. Anomaly Detection
Identify unusual or outlier data points
Example: Fraud detection, quality control

4. Generation
Learn to create new, realistic data samples
Example: Image synthesis, data augmentation

We'll explore four powerful algorithms that tackle these tasks.

Clustering: K-Means

Main Idea: Represent each cluster by its center (mean)



- Each cluster has a **center** (centroid) μ_k (marked with $\times$)
- Points belong to their **nearest** center
- Goal: Find centers that minimize total distance to assigned points

K-Means Algorithm

K-Means Algorithm

Input: Data $\{x_1, x_2, \ldots, x_n\}$ and number of clusters K

Initialize: Randomly place K cluster centers $\mu_1, \mu_2, \ldots, \mu_K$

Repeat until convergence:

1. **Assignment Step:** For each point x_i, assign to nearest center

$$c_i = \arg\min_{k=1,\ldots,K} \|x_i - \mu_k\|^2$$

(find which center is closest)

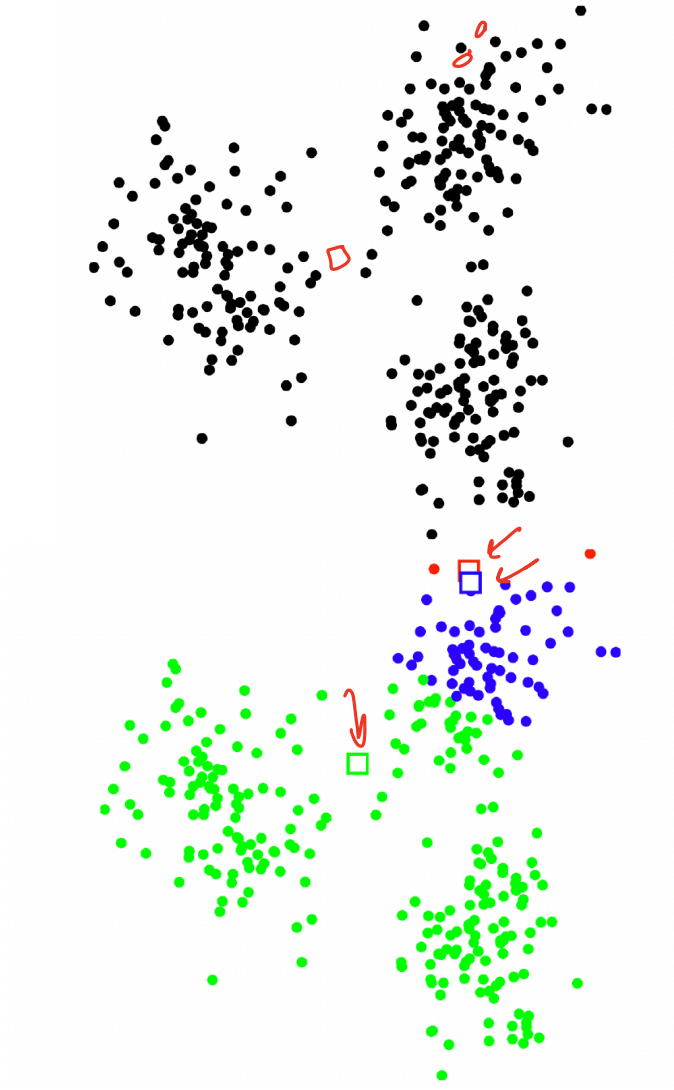
2. **Update Step:** Move each center to mean of assigned points

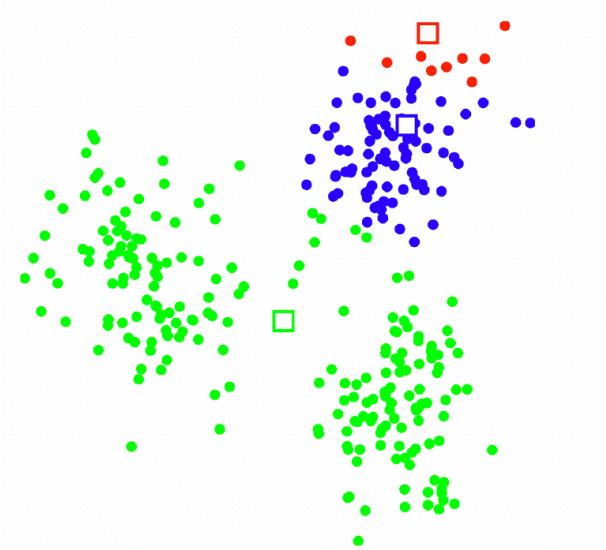
$$\mu_k = \frac{1}{|C_k|} \sum_{i \in C_k} x_i$$

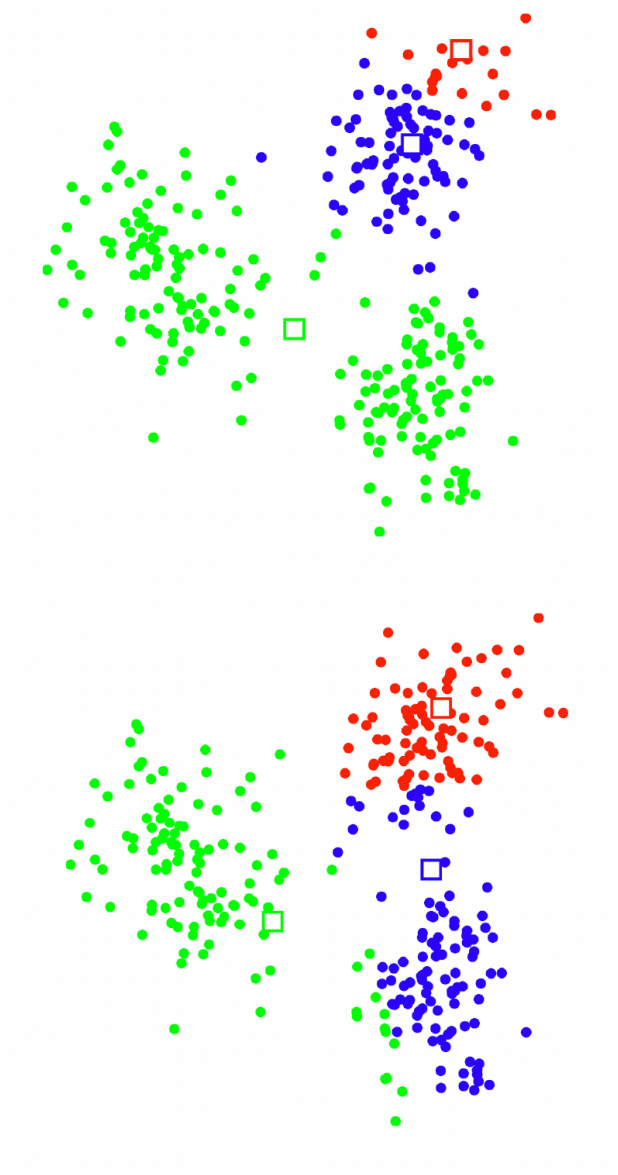
(average all points in cluster k)

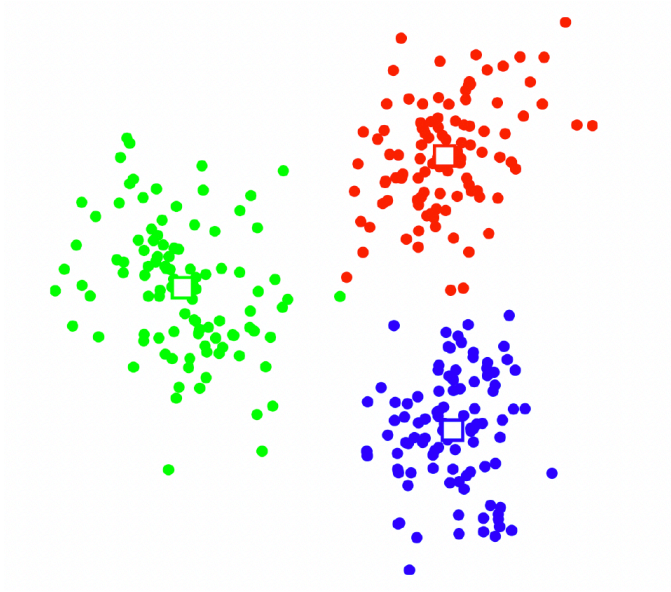
Stop when: Assignments don't change OR max iterations reached

K=3

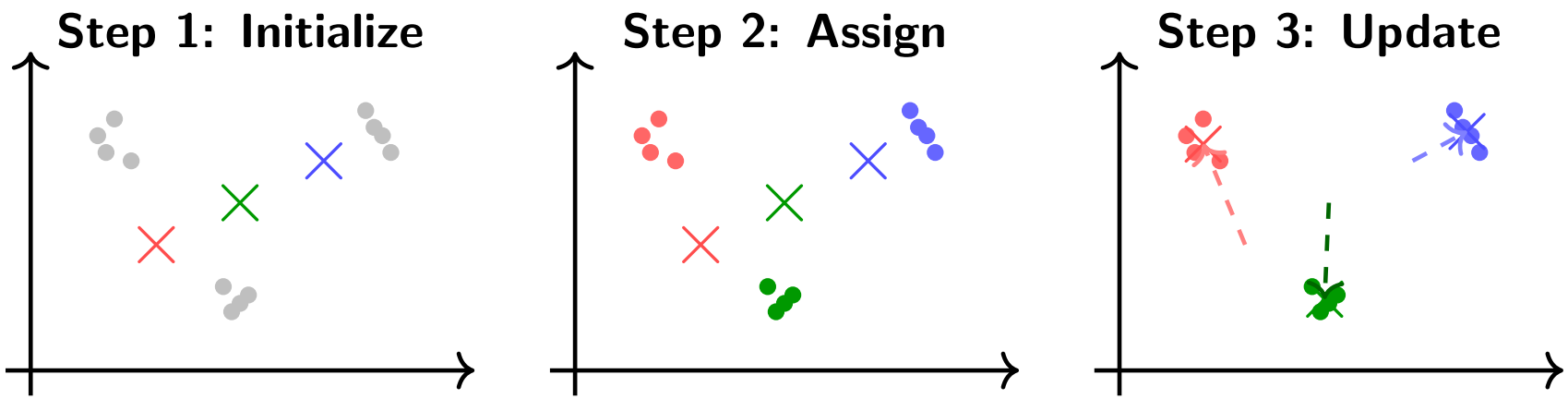








K-Means: Step-by-Step Example



Repeat steps 2-3 until centers stop moving (typically 10-100 iterations)

How to Choose K?

Problem: How many clusters should we use?

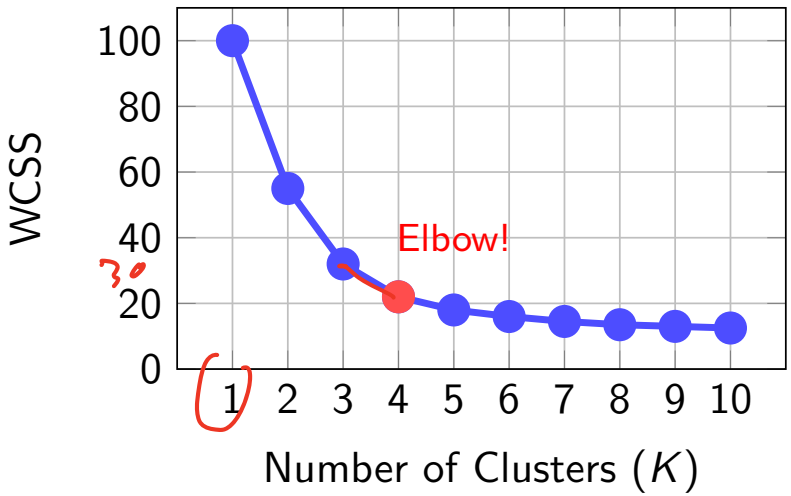
Elbow Method

Plot "within-cluster sum of squares" (WCSS) vs K

think of it as loss

$$= \text{WCSS} = \sum_{k=1}^{K} \sum_{i \in C_k} \|x_i - \mu_k\|^2$$

loss



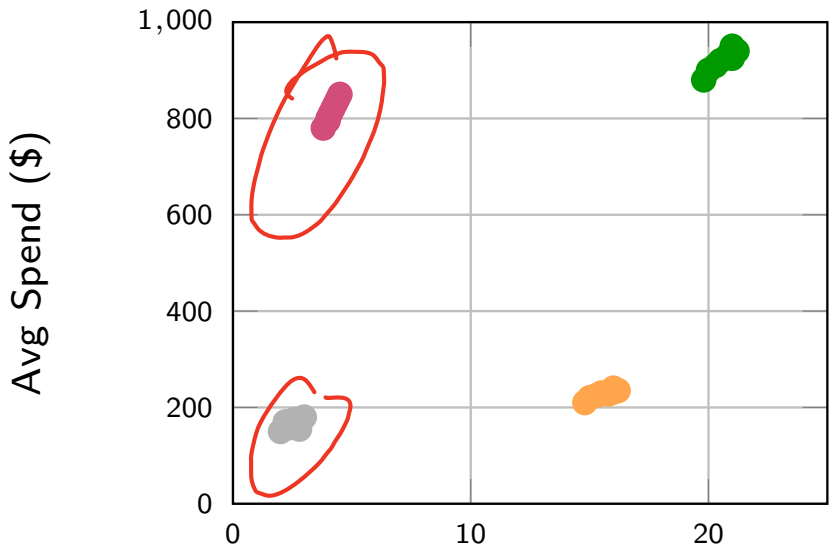
Look for the "elbow" where adding more clusters doesn't help much (in the above case it is 4)

Application 1: Customer Segmentation

Use case: Group customers for targeted marketing

Example: E-commerce Data

- Features: frequency, spend, recency
- Run K-Means with $K = 4$
- Interpret clusters



Discovered Segments:

Inactive
Low freq, low spend
Action: Re-engage

Bargain
High freq, low spend
Action: Discounts

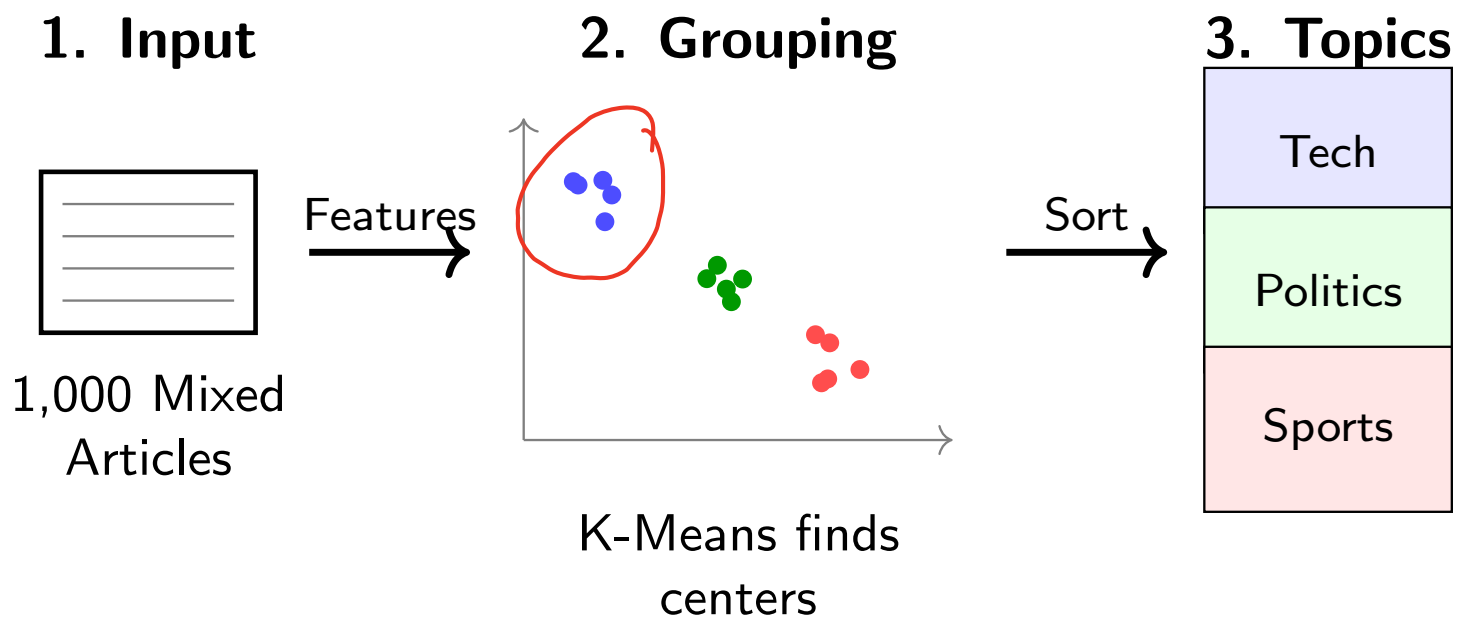
Big Spenders
Low freq, high spend
Action: Premium Service

VIP
High freq, high spend
Action: Loyalty Program

Application 2: Document Clustering

Topic discovery

Use case: Automatically organize news articles by topic.

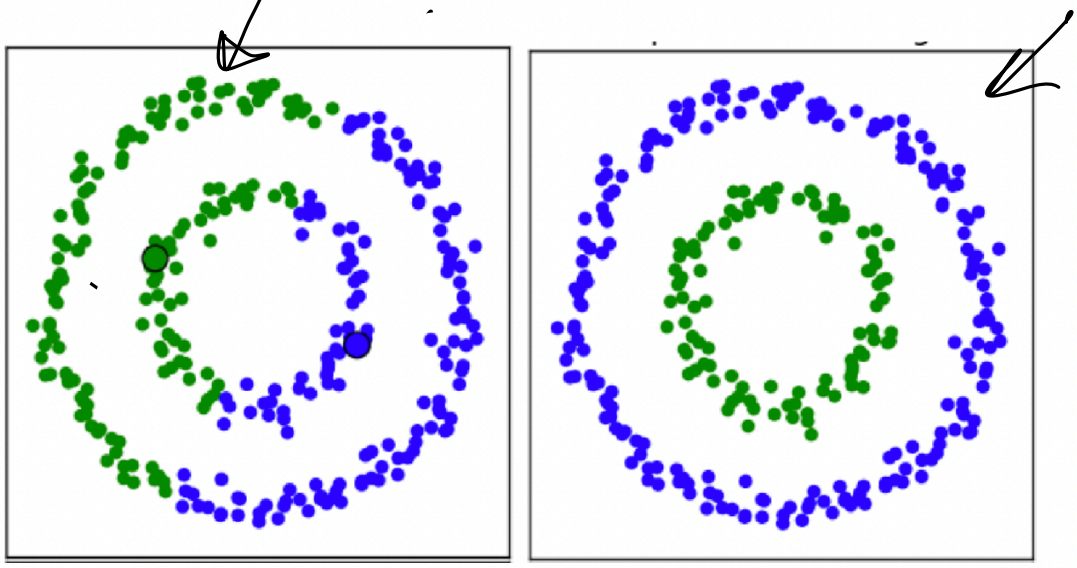


Process

- Convert text into numbers (Text Features).
- Similar stories appear close together in space.
- K-Means automatically groups them into topics.

Example: Google News grouping stories from different sources.

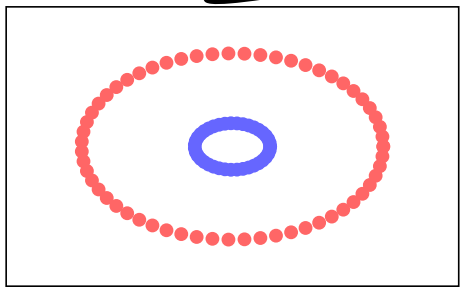
Can k-means fail?



When K-Means Fails

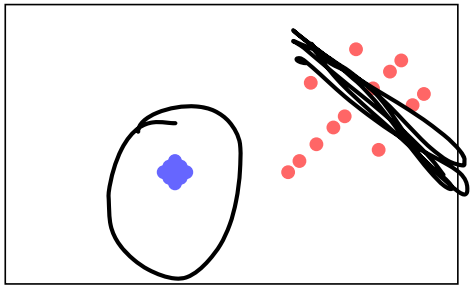
K-Means assumes spherical, equal-sized clusters

Problem 1: Non-spherical



Fails on concentric circles!

Problem 2: ~~Different sizes~~



Struggles with size differences!

Other Limitations

- Sensitive to outliers
- Must specify K in advance
- Random ~~initialization mat~~ters
- Bad results for high dimensional data

Alternatives: DBSCAN (density-based), Gaussian Mixture Models, Hierarchical clustering

The Curse of Dimensionality

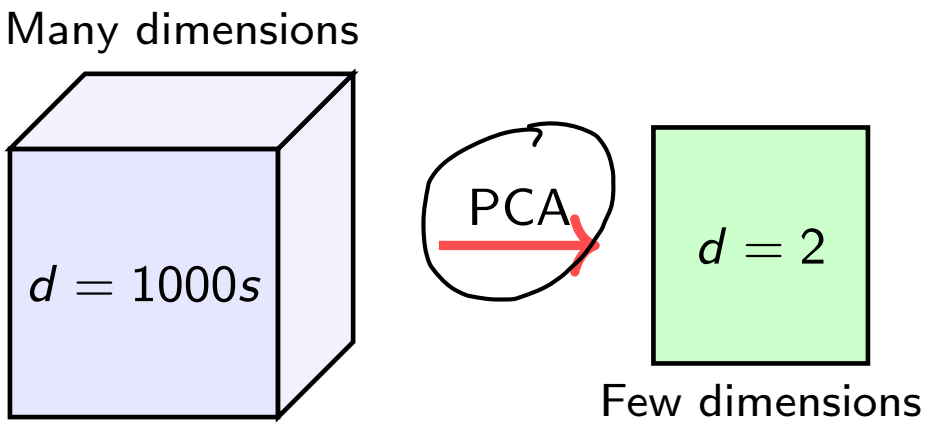
Real-world data is high-dimensional:

Examples:

- Images: $1000 \times 1000 = 1\text{M}$ pixels
- Text: 10,000+ words
- Genomics: 20,000+ genes
- Sensors: 100+ measurements

Problems:

- Hard to visualize
- Slow to compute
- Lots of redundancy
- Noisy measurements



Solution: Find a lower-dimensional representation while keeping important information (Dimensionality Reduction)

What is PCA?

Principal Component Analysis (PCA) is a dimensionality reduction algorithm that finds the most important directions in your data.

Core Idea

Instead of using original features, create **new features** (principal components) that:

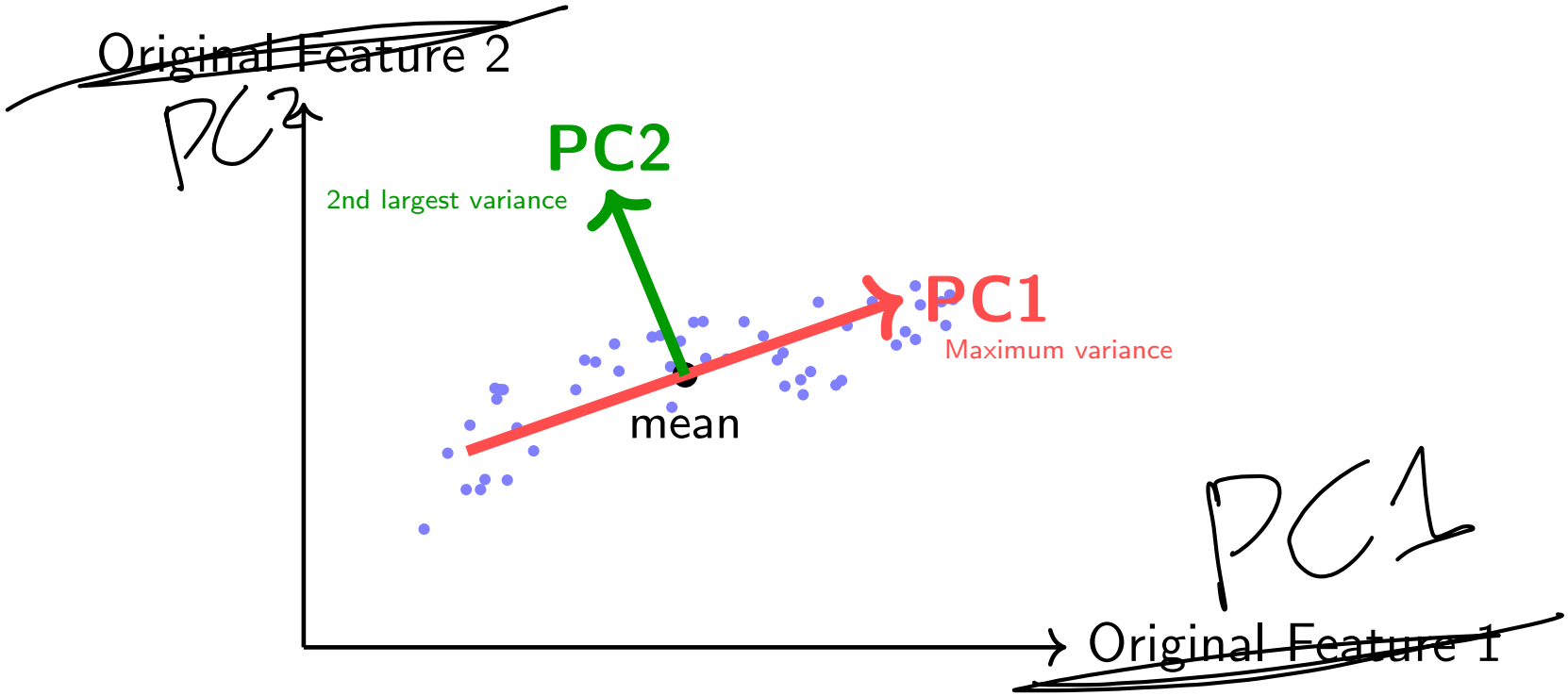
- Capture maximum variance
- Are uncorrelated with each other
- Are ranked by importance

Then keep only the top few components!

Original Data 784 features (correlated, noisy)	$\xrightarrow{\text{PCA}}$	New Data 50 components (uncorrelated, clean)

PCA Intuition: Finding the Best Directions

Goal: Find directions where data varies the most.



- PC1: Direction with most spread
- PC2: Perpendicular to PC1, next most spread
- PC3, PC4, ... : Each perpendicular to all previous ones

How Does PCA Work? (Part 1)

Step 1: Prepare the Data

1. Center the Data

Shift the data so the center is at the origin (0,0).

$$X_{\text{centered}} = X - \bar{X}$$

(Subtract the mean from every feature)

2. Compute Covariance Matrix

Calculate how features vary with respect to each other.

Symmetric Matrix

$$\boxed{C = \frac{1}{n} X_{\text{centered}}^{\top} X_{\text{centered}}} =$$

$Cov(X_1, X_2)$ $Cov(X_1 X_3)$

σ_1^2 σ_2^2 σ_3^2

(Finds correlations between features)

How Does PCA Work? (Part 2)

Step 2: Find Directions & Project

SVD

3. Find Principal Components

Calculate **Eigenvectors** and **Eigenvalues** of the covariance matrix C.

- **Eigenvectors:** The directions of the new axes.
- **Eigenvalues:** The amount of variance (information) along those axes.

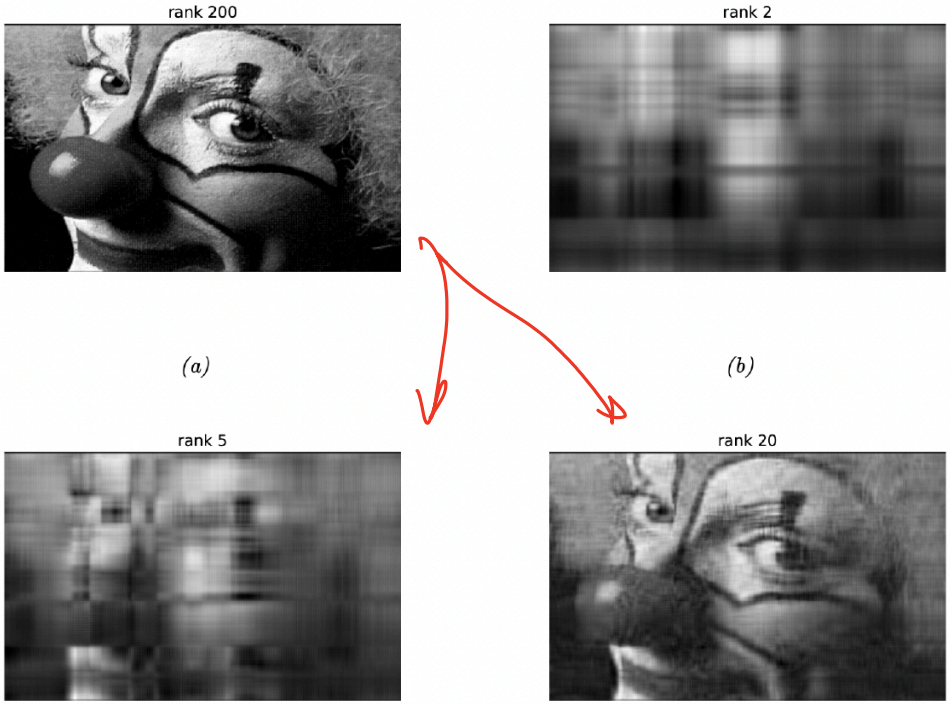
4. Select & Project

Pick the top k eigenvectors with the largest eigenvalues and transform the data.

$$Z = X_{\text{centered}} \cdot \boxed{V_k}$$

(Reduces data from d dimensions $\rightarrow$ k dimensions)

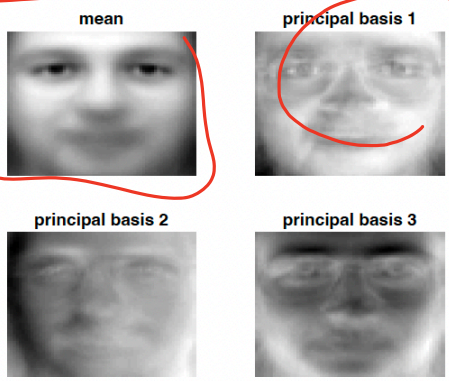
Image Compression



(a) (b) (c) (d)

(a)

Centered data



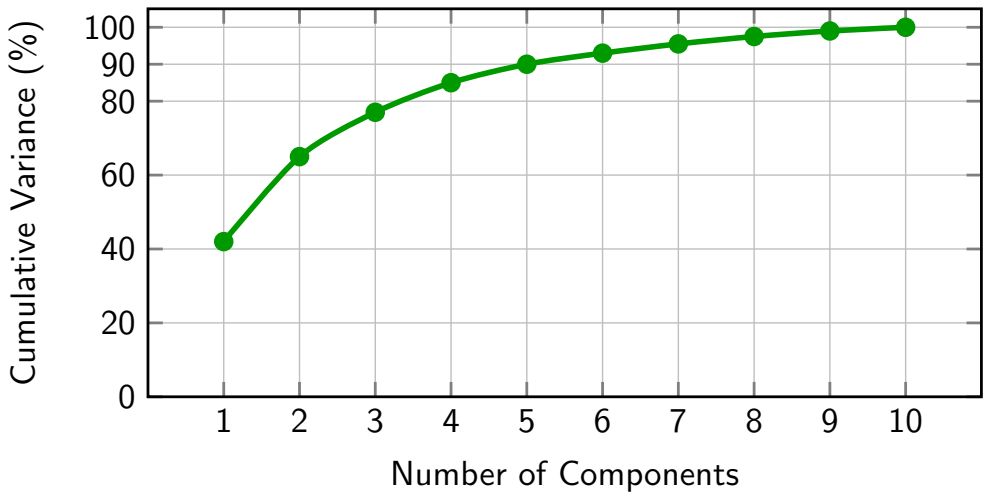
(b)

How Many Components to Keep?

Key question: How many components are enough?

Cumulative Variance Explained

(The most common method for selecting K)



Rule of Thumb: Choose the smallest K that preserves **80–95%** of the total variance.

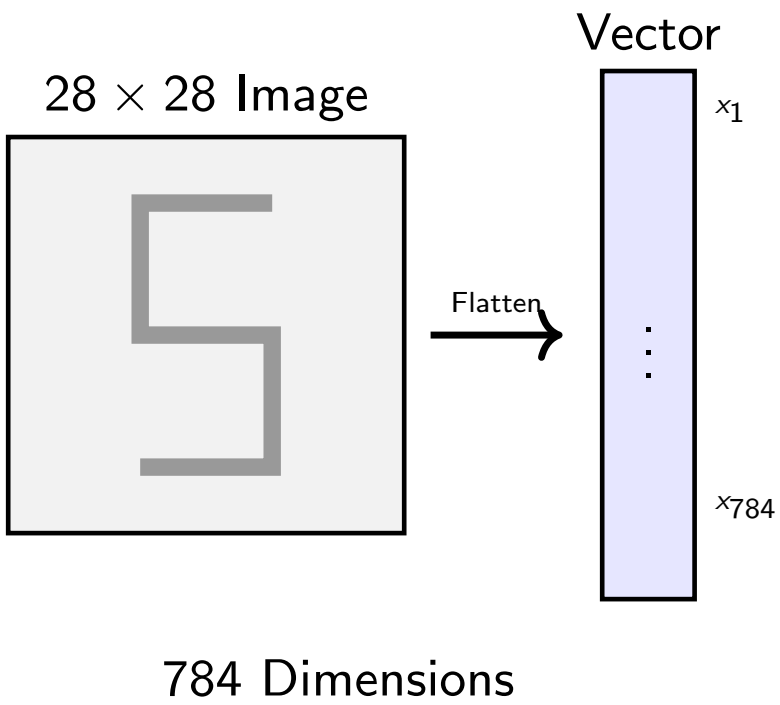
Application 1: Data Visualization

The Data: MNIST Digits, 70,000 handwritten digits (0–9).

The Challenge:

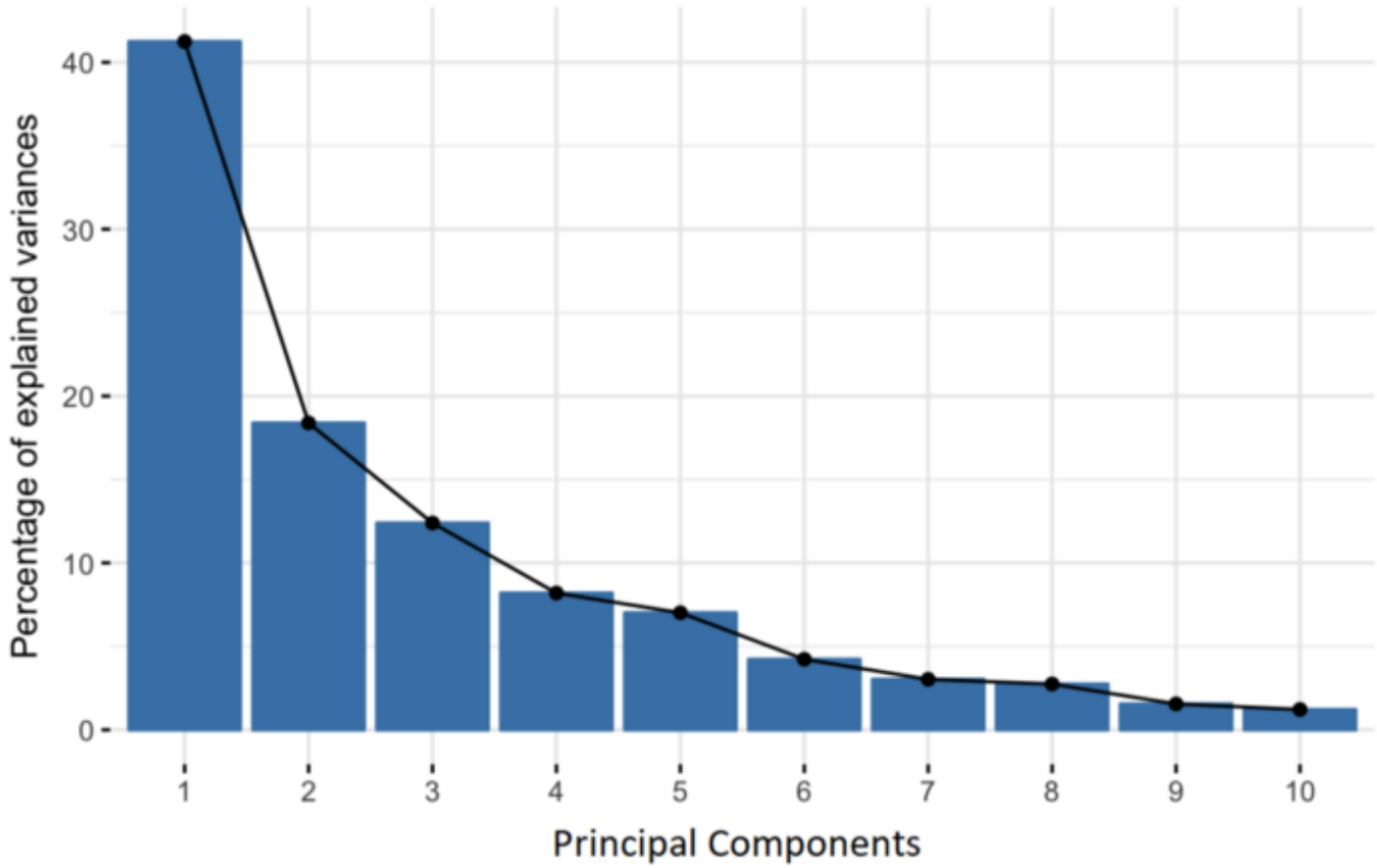
- Each image is 28×28 pixels.
- Total features: $28 \times 28 = \mathbf{784}$ dimensions!
- We cannot "see" in 784 dimensions.

Question: Can we compress this to just **2D** to see how the digits relate?



Application 1: Data Visualization

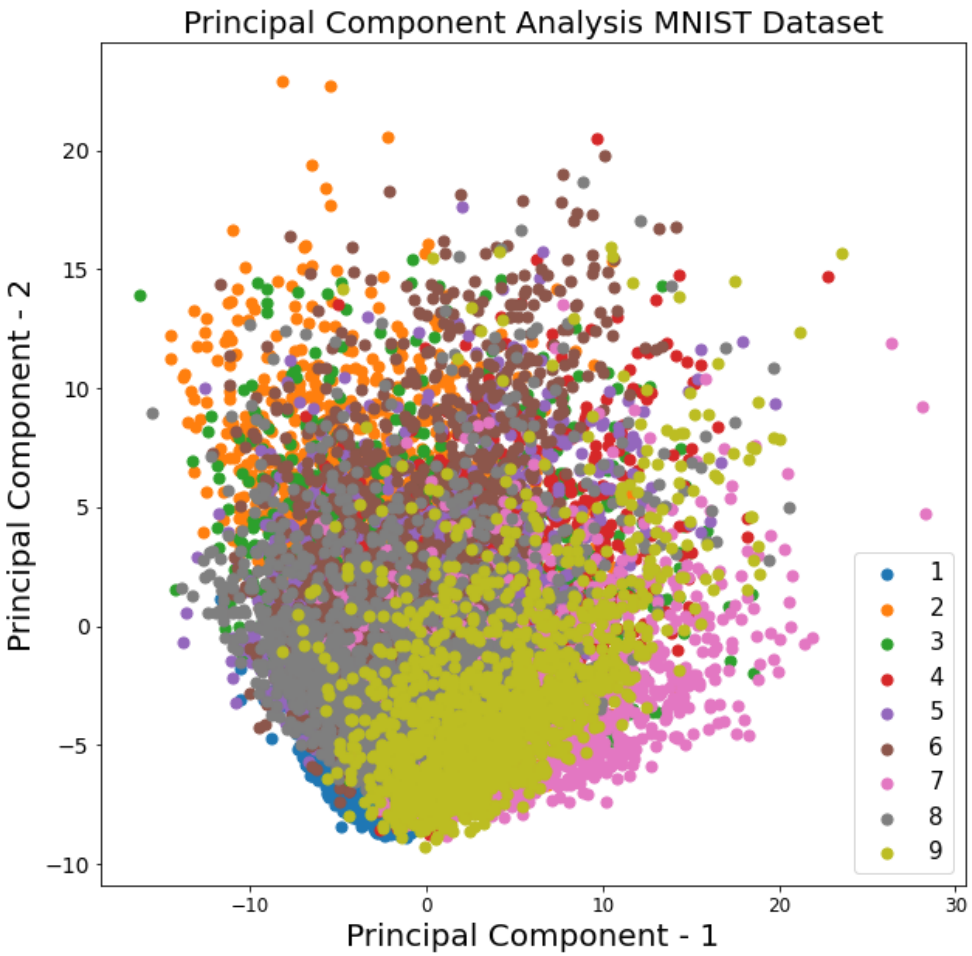
Applying PCA: We project the 784 dimensions down to the top 2 Principal Components.



Application 1: Data Visualization

Is this the best visualization?

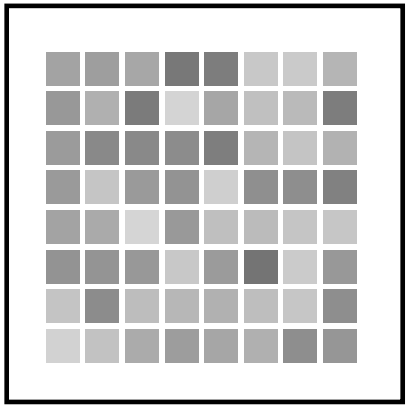
- It captures some structure, but points overlap heavily.
- **Reason:** PCA is **linear**, it cannot unfold complex, curved structures.
- PCA is mostly used for compression. We will cover a better visualization algorithm shortly.



Application 2: Data Compression

Use case: Store data more efficiently

Original



$28 \times 28 = 784$ values

PCA
50 comps

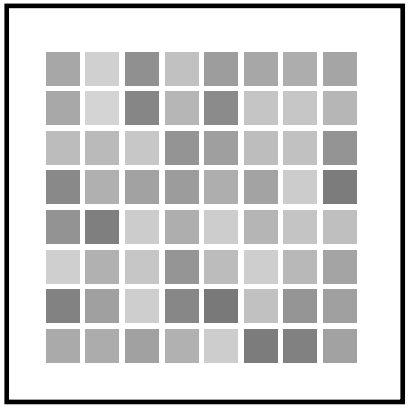
Compressed

[0.42, -1.3, 0.87, ...]
50 values

93% smaller

Reconstruct

Reconstructed



Similar to original
(but with small error)

More components = better reconstruction, less compression

10 PCs	**50 PCs**	**200 PCs**
99% compression	93% compression	75% compression
(blurry)	(good)	(near perfect)

PCA Limitations

$X_{centered}$

PCA Limitations:

- **Linear only**: Finds linear combinations of features
- **Sensitive to scale**: Must standardize data first → finding scaled data
- **Not Interpretable**: PCs are combinations of all features
- **Outliers**: Can distort principal components

Let's have a look at a better algorithm for high dimensional data visualization...

t-SNE: Why Do We Need It?

PCA is great... but it's linear. Many datasets have **non-linear** structure.

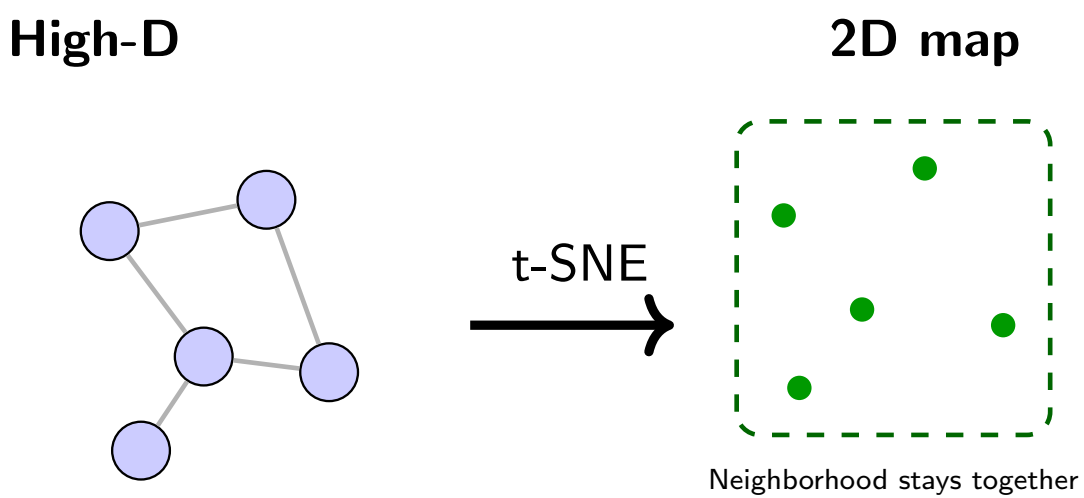
Problem

- High-dimensional data can be hard to visualize
- PCA may **mix** classes if the separation is non-linear
- We mainly want a **good 2D plot** for exploration

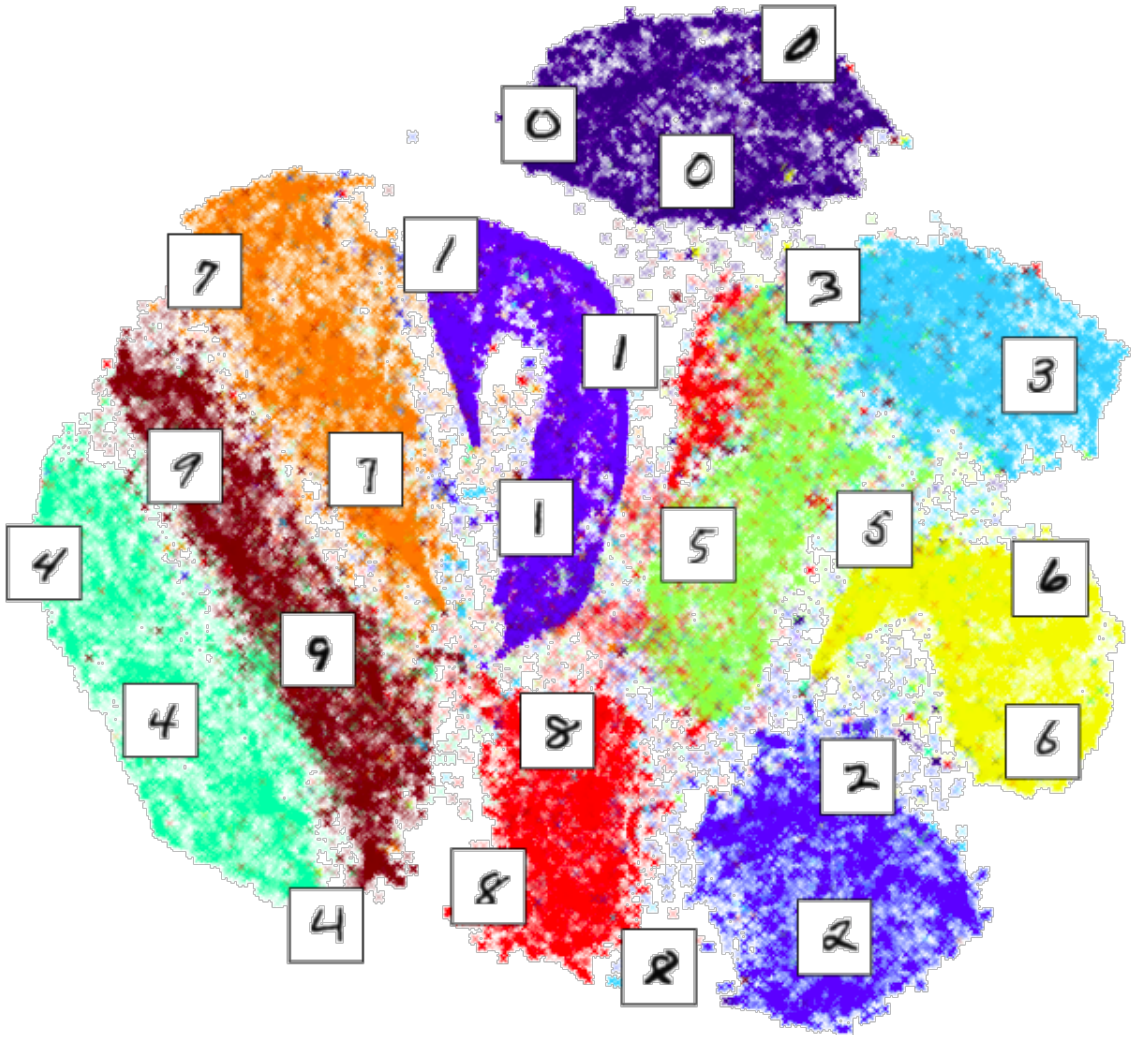
t-Distributed Stochastic Neighbor Embedding (t-SNE)

Main Idea

t-SNE tries to build a 2D map where: neighbors in high-D remain neighbors in 2D.



Example: Visualizing MNIST via t-SNE

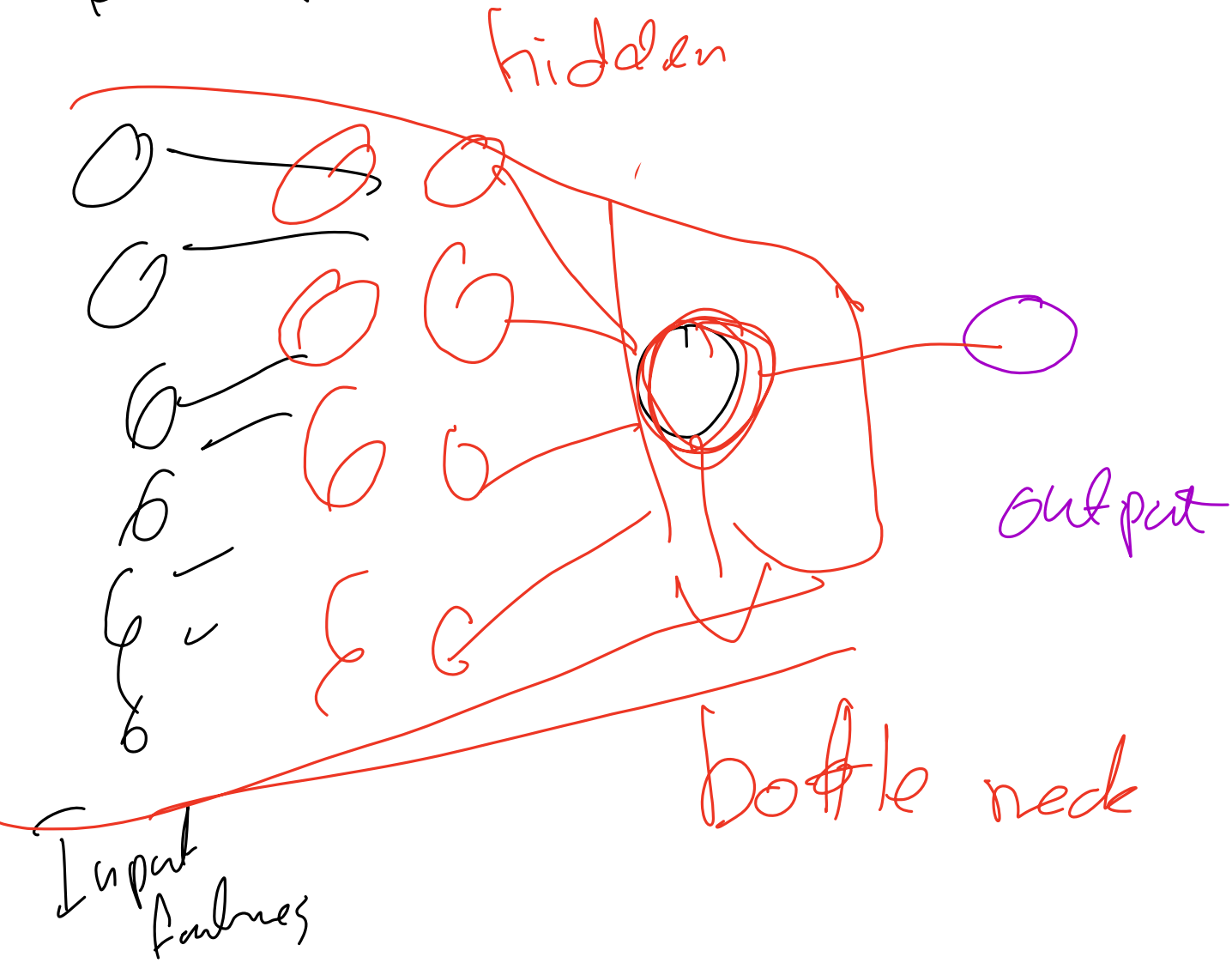


This is much better than PCA! We can see how similar digits are grouped together, while different ones are far from each other.

We have covered classical algorithms like K-Means and PCA.

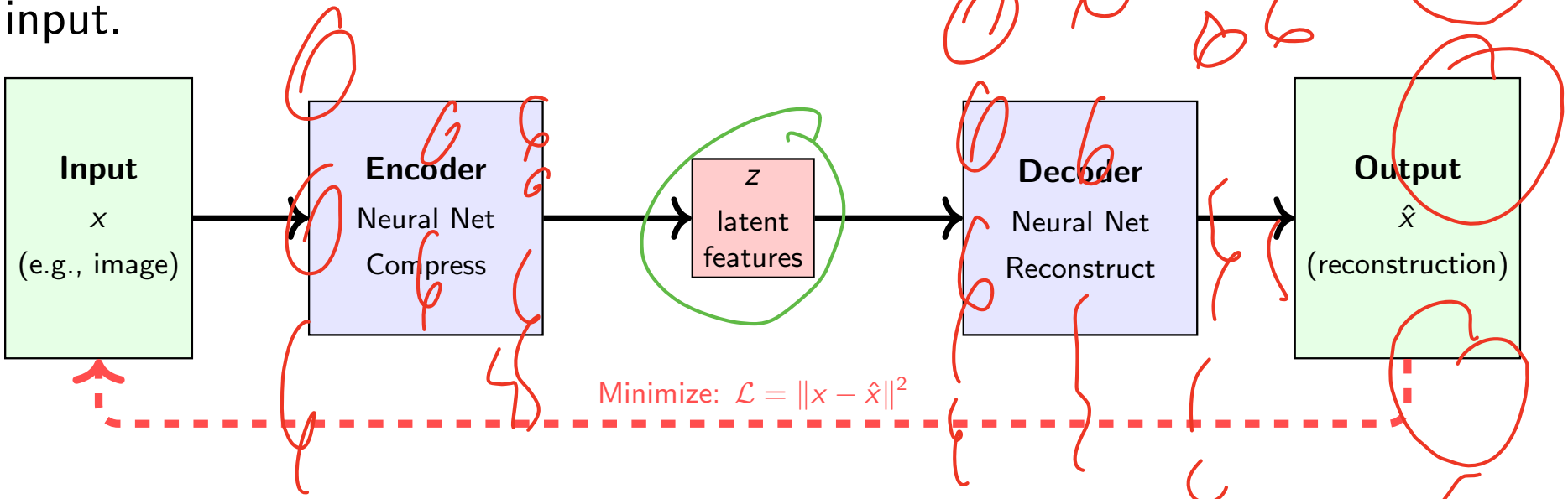
Now, let's explore a powerful Neural Network architecture designed for unsupervised learning...

DNN = DL



What is an Autoencoder?

Autoencoder: a type of neural network that learn to compress data into a compact form and then reconstruct it to match the original input.



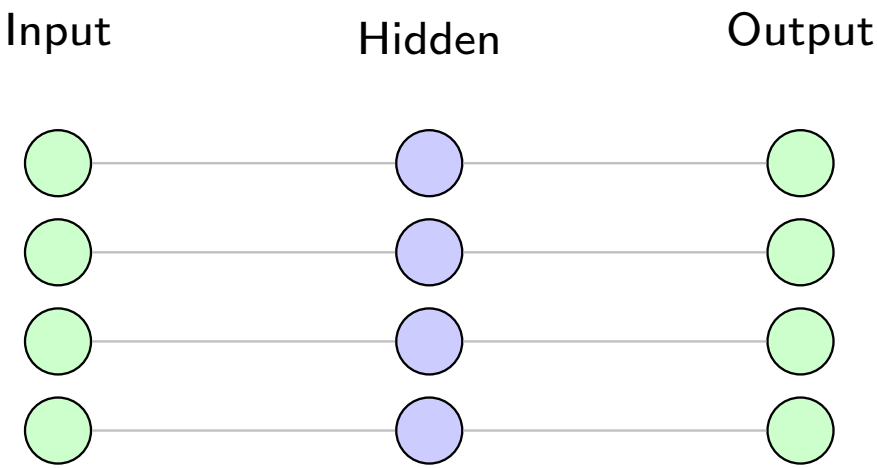
The trick: Force information through a narrow **bottleneck** z.

This forces the network to learn compressed, meaningful representations!

Why Does the Bottleneck Work?

What if there's no bottleneck?

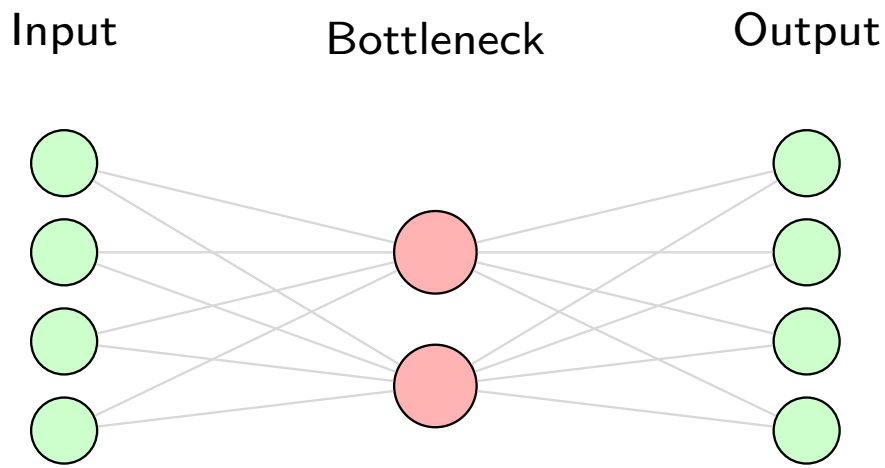
Without Bottleneck



Network can just copy:
$h_i = x_i$, $\hat{x}_i = h_i$

Learns nothing useful!

With Bottleneck



Must compress 4D $\rightarrow$ 2D
Forces learning of structure!

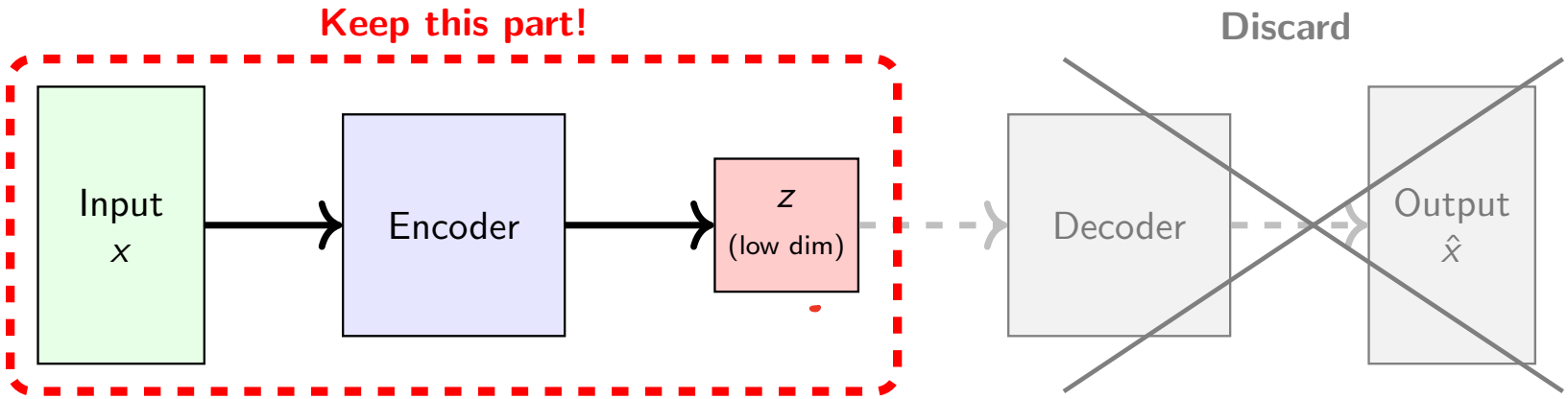
Learns meaningful features!

Application 1: Dimensionality Reduction

How to use an Autoencoder for compression:

input 784

output 784

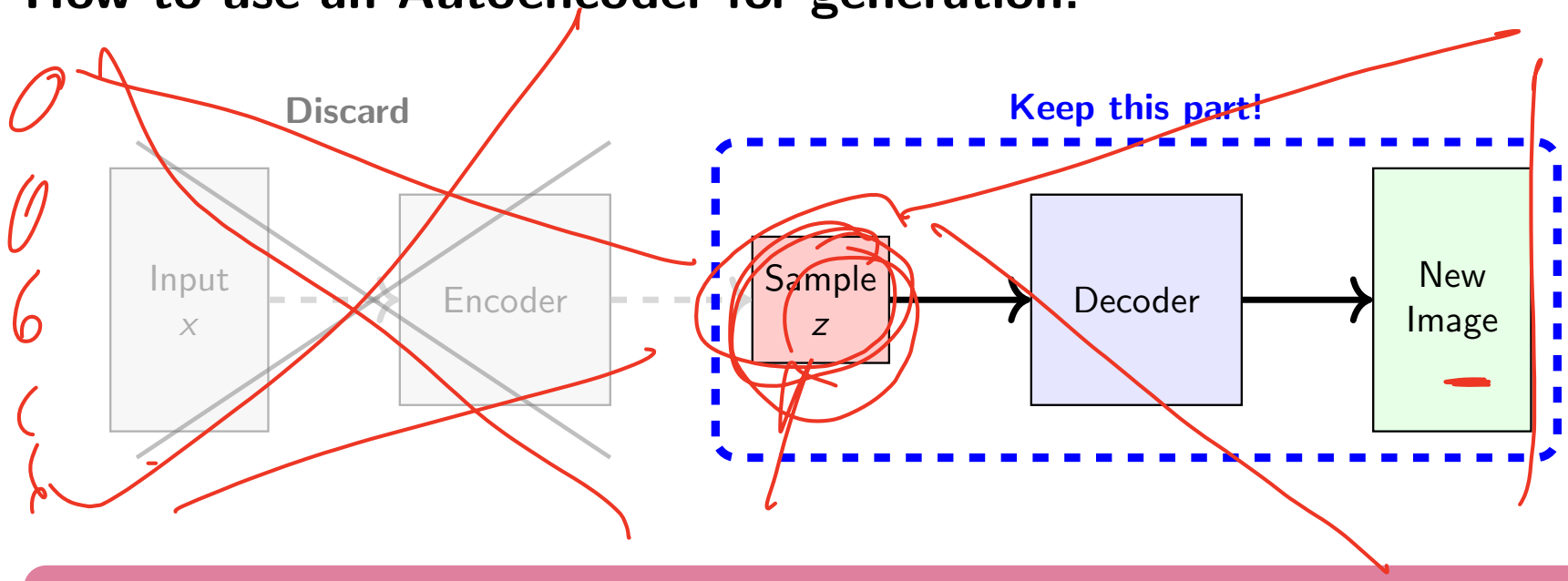


The Process

1. **Train** the full network to reconstruct the input ($x \approx \hat{x}$).
2. **Discard** the Decoder (it's only needed for training).
3. **Use the Encoder** to map high-dimensional data x to low-dimensional code z.

Application 2: Image Generation

How to use an Autoencoder for generation:

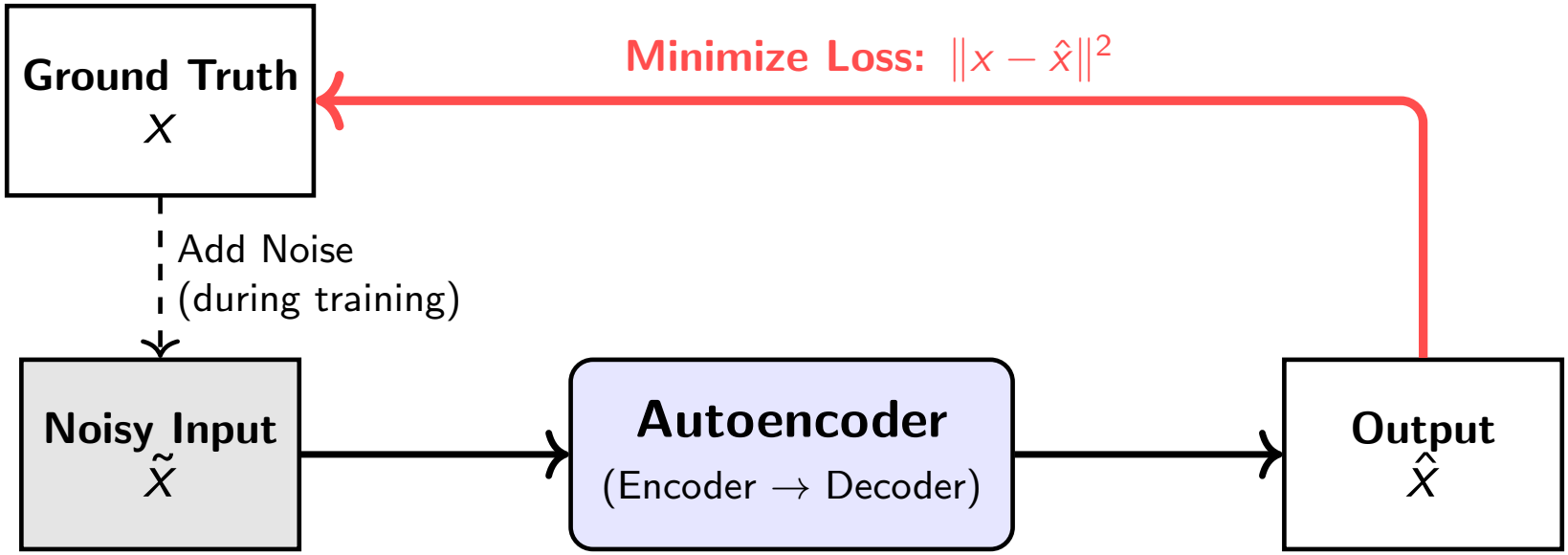


The Process

1. **Train** the full network on images to learn features.
2. **Discard** the Encoder.
3. **Sample** a random vector z (pick random numbers).
4. **Generate** a brand new image by running z through the Decoder.

Application 3: Denoising Autoencoders

Idea: Train the network to recover the original signal from corrupted input.



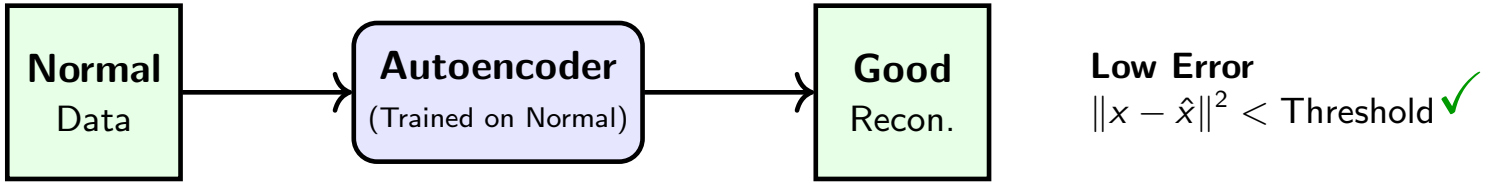
How it works

- Take clean image x.
- Corrupt it to get $\tilde{x}$.
- Force AE to map $\tilde{x} \to x$.

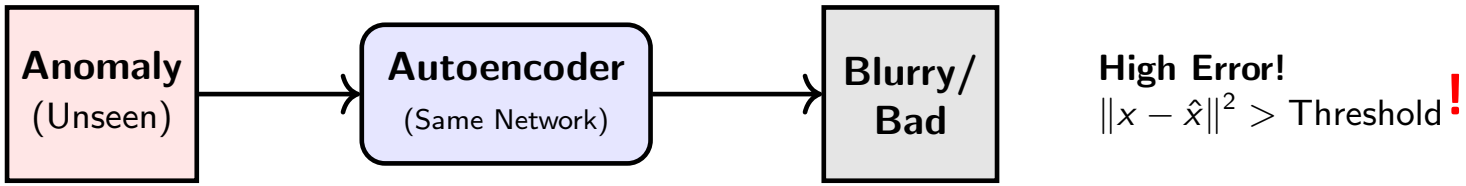
Application 4: Anomaly Detection

Concept: The network learns to reconstruct "Normal" data perfectly. When it sees an anomaly, it fails to reconstruct it.

1. Training / Normal Operation



2. Detection Phase



Real-World Use Cases

- **Credit Card Fraud:** Normal transactions reconstruct well, theft looks weird.
- **Manufacturing:** Detect defective parts on an assembly line.

References

- Aurélien Géron, *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*
- Andrew Ng, *Machine Learning Specialization* (Coursera/DeepLearning.AI)

Slides contributed by Mohamed Eltayeb