L05: PCA & t-SNE

Deep Dive: Theory, Implementation, and Applications

Methods and Algorithms – MSc Data Science

Part 1: PCA Foundations

Principal Component Analysis (PCA)

- Find orthogonal directions of maximum variance
- Project data onto these directions
- Reduce dimensions while preserving information

Key Properties:

- Linear transformation
- Components are uncorrelated
- Reversible (can reconstruct original data)

PCA: one of the most fundamental tools in data science

Mathematical Foundation

Covariance Matrix:

$$\Sigma = \frac{1}{n-1} X^T X \quad \text{(centered data)}$$

Eigendecomposition:

$$\Sigma v = \lambda v$$

where v = eigenvector (principal direction), λ = eigenvalue (variance)

Projection:

$$Z = XW_k \quad \text{where } W_k = [v_1, v_2, \ldots, v_k]$$

Eigenvalues tell us how much variance each component captures

Variance Explained

Proportion of Variance:

$$\text{Explained Variance Ratio}_i = \frac{\lambda_i}{\sum_{j=1}^{p} \lambda_j}$$

Cumulative Variance:

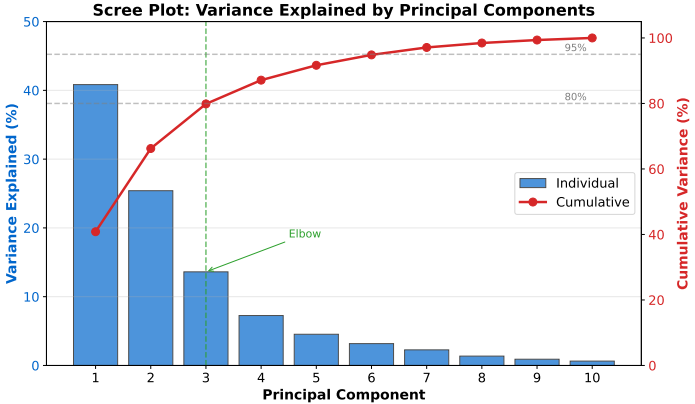
$$\text{Cumulative}_k = \sum_{i=1}^{k} \frac{\lambda_i}{\sum_{j=1}^{p} \lambda_j}$$

Rules of thumb for choosing k:

- Keep 80-95% of total variance
- Use scree plot "elbow" method
- Kaiser criterion: keep components with $\lambda > 1$

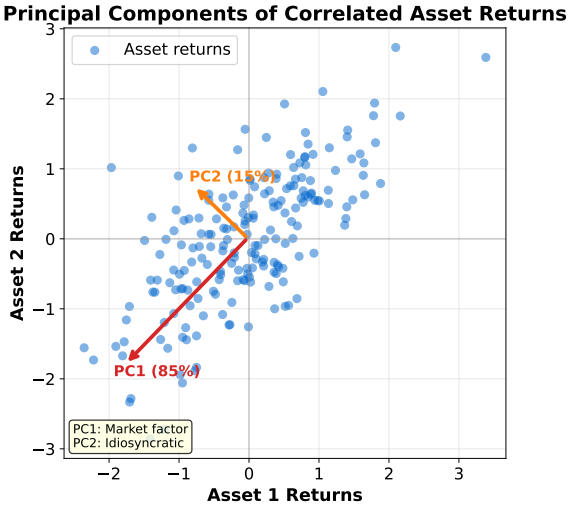
Balance dimensionality reduction with information preservation

Scree Plot



Look for the "elbow" where variance explained drops off

Principal Components Visualization



PC1 captures the dominant trend, PC2 the residual variation

Reconstruction

From k components back to original space:

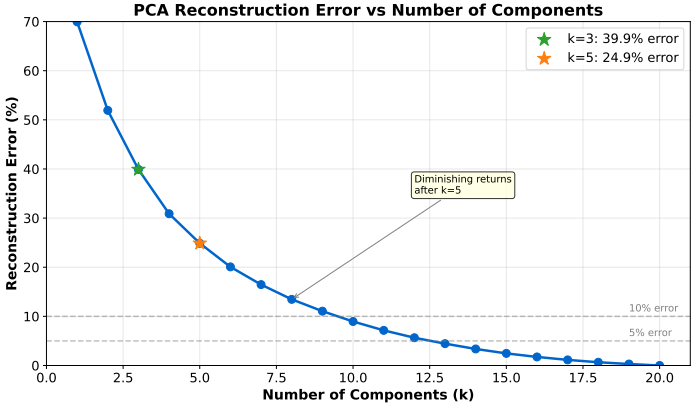
$$\hat{X} = ZW_k^T = XW_kW_k^T$$

Reconstruction Error:

$$\text{Error} = ||X - \hat{X}||_F^2 = \sum_{i=k+1}^{p} \lambda_i$$

Reconstruction error = sum of discarded eigenvalues

Reconstruction Error vs Components



Adding more components always reduces error (but diminishing returns)

Part 2: PCA in Finance

Portfolio Risk Decomposition:

- PC1 often represents "market factor"
- PC2-3 may capture sector/size factors
- Higher PCs: idiosyncratic risk

Applications:

- Risk factor modeling
- Dimensionality reduction for trading signals
- Noise reduction in time series
- Feature extraction for ML models

PCA reveals latent structure in financial data

PCA Limitations

When PCA Falls Short:

- Non-linear relationships (curved manifolds)
- Cluster structure not aligned with variance
- Discrete or categorical data
- Outliers heavily influence results

Solutions:

- Kernel PCA (non-linear)
- Robust PCA (outlier-resistant)
- t-SNE/UMAP (for visualization)

PCA assumes linear structure and Gaussian-like distributions

Part 3: t-SNE Introduction

t-Distributed Stochastic Neighbor Embedding

- Non-linear dimensionality reduction
- Optimized for visualization (2D/3D)
- Preserves local neighborhood structure

Key Idea:

- Convert distances to probabilities
- In high-D: Gaussian similarities
- In low-D: t-distribution similarities
- Minimize KL divergence between distributions

t-SNE: visualization method, NOT for preprocessing

t-SNE: Mathematical Formulation

High-dimensional similarity:

$$p_{j|i} = \frac{\exp(-||x_i - x_j||^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-||x_i - x_k||^2/2\sigma_i^2)}$$

Low-dimensional similarity (t-distribution):

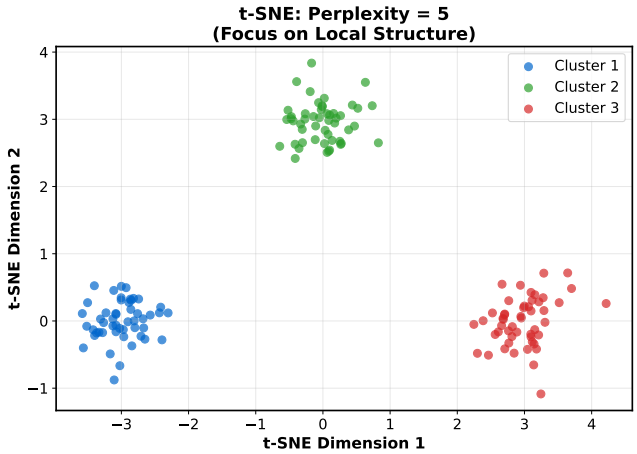
$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k \neq l}(1 + ||y_k - y_l||^2)^{-1}}$$

Objective: Minimize KL divergence

$$KL(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

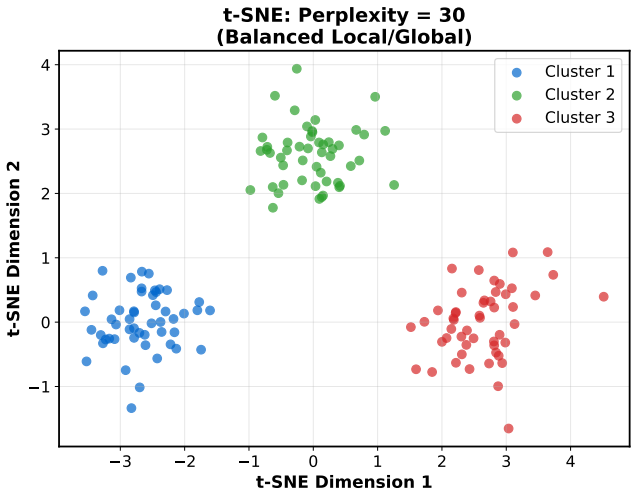
t-distribution has heavier tails, allowing better separation in low-D

Perplexity: Low (Local Focus)



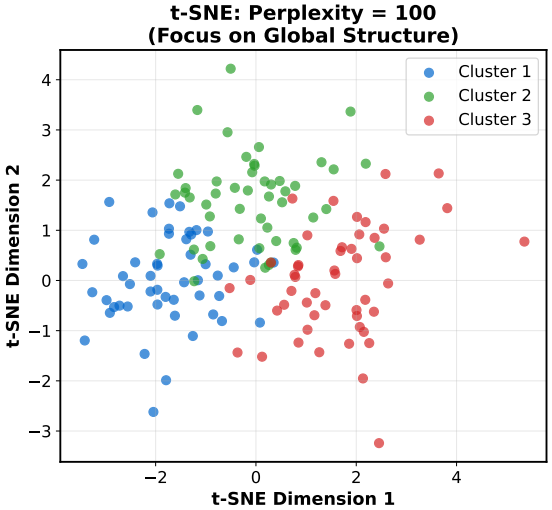
Low perplexity (5): tight clusters, focus on nearest neighbors only

Perplexity: Default (Balanced)



Default perplexity (30): balanced local and global structure

Perplexity: High (Global Focus)



High perplexity (100): more spread, clusters may merge

Perplexity Guidelines

Perplexity controls the balance between local and global structure:

- Low perplexity (5-10): Focus on very local structure
- Medium perplexity (30-50): Balanced (default)
- High perplexity (100+): More global structure

Guidelines:

- Should be smaller than number of points
- Larger datasets can use higher perplexity
- Run multiple perplexities to validate findings

Results can vary significantly with perplexity choice

t-SNE Caveats

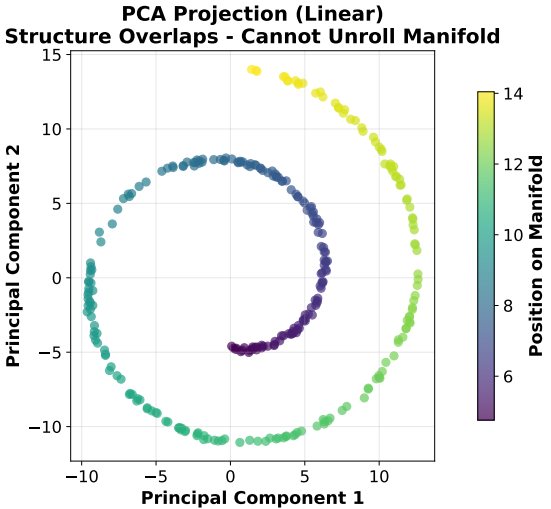
Important Limitations:

- Non-deterministic (run multiple times)
- Cluster sizes are not meaningful
- Distances between clusters are not meaningful
- Slow for large datasets ($O(n^2)$)

Best Practices:

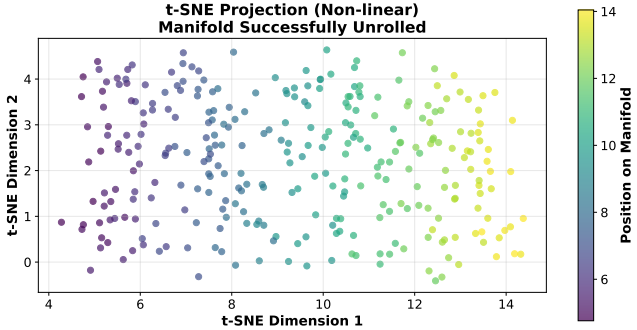
- Use PCA first to reduce to 30-50 dims
- Run multiple times with different seeds
- Don't over-interpret cluster sizes/distances
- Use for exploration, not final conclusions

t-SNE shows IF clusters exist, not HOW they relate



PCA (linear) cannot unroll the Swiss roll - structure overlaps

t-SNE on Non-linear Manifolds



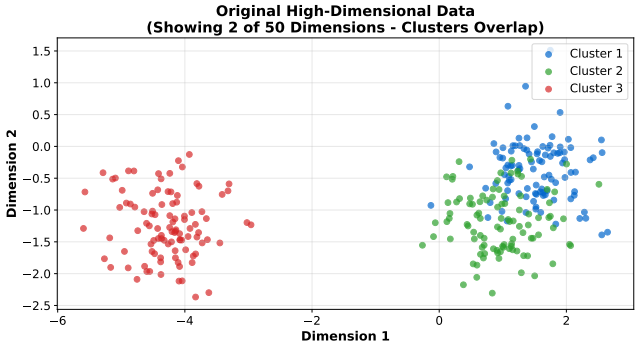
t-SNE (non-linear) successfully unrolls the manifold structure

Comparison Table

Aspect	PCA	t-SNE
Type	Linear	Non-linear
Speed	Fast $O(np^2)$	Slow $O(n^2)$
Deterministic	Yes	No
Preserves	Global variance	Local neighbors
Reversible	Yes	No
Use for ML	Yes (preprocessing)	No
Visualization	Okay	Excellent

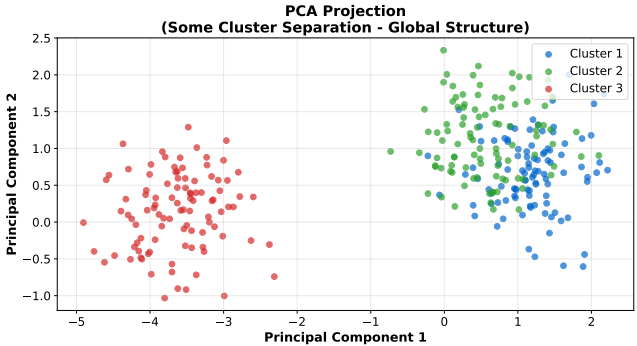
Use PCA for preprocessing, t-SNE for visualization only

Cluster Preservation: Original Data



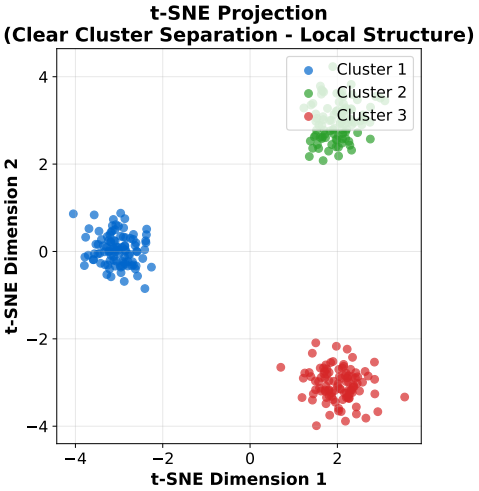
High-dimensional data (50 dims): clusters overlap when viewed in 2D

Cluster Preservation: PCA Projection



PCA finds directions of max variance - some cluster separation

Cluster Preservation: t-SNE Projection



t-SNE preserves local structure - clear cluster separation

When to Use Which

Use PCA When:

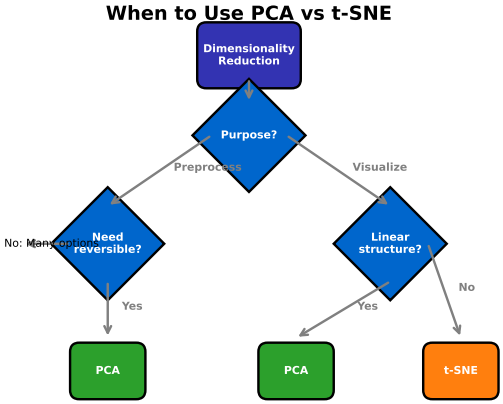
- Preprocessing for ML (reduce features)
- Linear relationships expected
- Need reversibility (reconstruction)
- Speed matters

Use t-SNE When:

- Visualizing high-dimensional data
- Looking for cluster structure
- Non-linear manifolds expected
- Exploratory analysis

Often use both: PCA first to 30-50 dims, then t-SNE for visualization

Decision Framework



PCA: Fast, linear, reversible, for preprocessing

t-SNE: Slow, non-linear, visualization only, preserves local structure

Consider purpose: preprocessing (PCA) vs visualization (t-SNE)

Part 5: Implementation

PCA in scikit-learn:

- `PCA(n_components=k)`: Keep k components
- `PCA(n_components=0.95)`: Keep 95% variance
- `pca.explained_variance_ratio_`: Variance per component
- `pca.inverse_transform()`: Reconstruct original

t-SNE in scikit-learn:

- `TSNE(n_components=2, perplexity=30)`
- Always normalize data first
- Consider PCA preprocessing for speed

Standardize data before PCA; normalize before t-SNE

UMAP: Modern Alternative

Uniform Manifold Approximation and Projection

- Faster than t-SNE
- Better preserves global structure
- Can embed new points (unlike t-SNE)
- Hyperparameters: n_neighbors, min_dist

When to use UMAP:

- Large datasets (faster than t-SNE)
- Need to embed new data points
- Want more preserved global structure

UMAP often preferred over t-SNE in modern practice

Summary

PCA:

- Linear, fast, reversible
- Use for preprocessing and feature extraction
- Choose k by variance explained or elbow

t-SNE:

- Non-linear, slow, visualization-only
- Excellent for exploring cluster structure
- Don't interpret distances or sizes literally

Common Pipeline: Standardize $\rightarrow$ PCA (30-50) $\rightarrow$ t-SNE (2D)

Next: Embeddings and Reinforcement Learning

References

Textbooks:

- James et al. (2021). *ISLR*, Chapter 12: Unsupervised Learning
- Hastie et al. (2009). *ESL*, Chapter 14: Unsupervised Learning

Original Papers:

- Pearson (1901). On Lines and Planes of Closest Fit
- van der Maaten & Hinton (2008). Visualizing Data using t-SNE
- McInnes et al. (2018). UMAP

Documentation:

- scikit-learn: `sklearn.decomposition.PCA`
- scikit-learn: `sklearn.manifold.TSNE`

t-SNE paper: one of the most influential visualization papers