Methods and Algorithms

Spring 2026

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

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:

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

Eigenvalues tell us how much variance each component captures

Proportion of Variance:

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

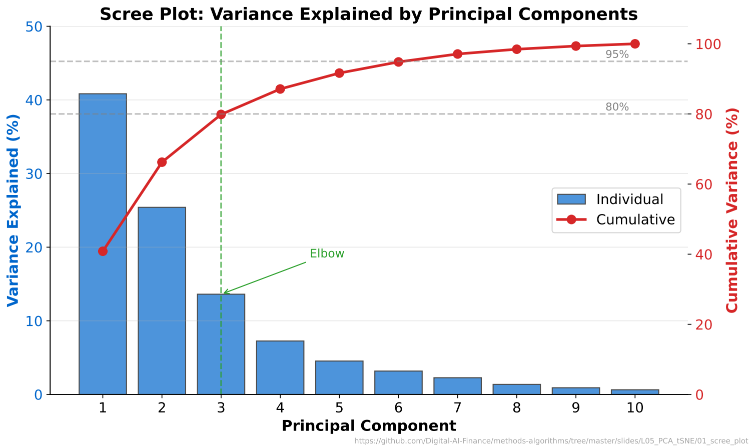
Cumulative Variance:

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

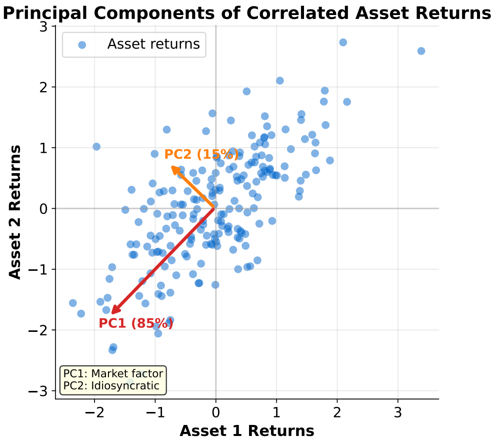
Rules of thumb for choosing k:

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

Balance dimensionality reduction with information preservation



Look for the "elbow" where variance explained drops off



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/02_principal_components

PC1 captures the dominant trend, PC2 the residual variation

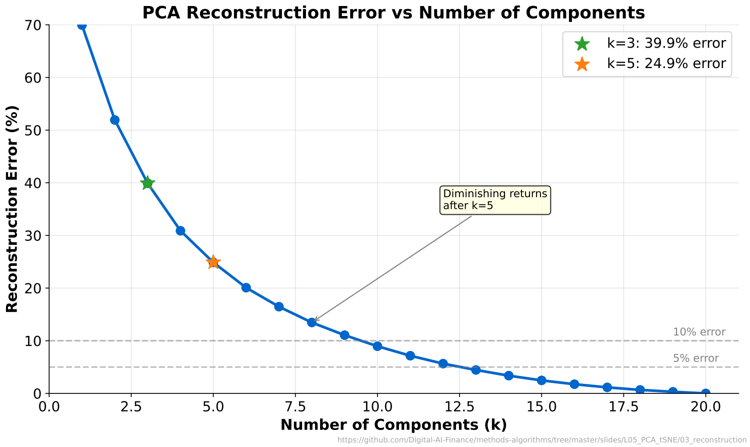
From k components back to original space:

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

Reconstruction Error:

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

Reconstruction error = sum of discarded eigenvalues



Adding more components always reduces error (but diminishing returns)

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

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

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

High-dimensional similarity:

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

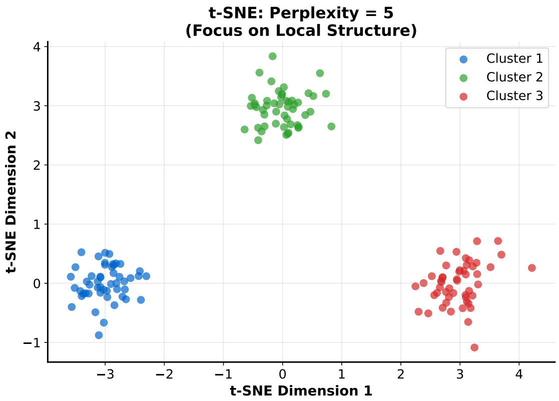
Low-dimensional similarity (t-distribution):

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

Objective: Minimize KL divergence

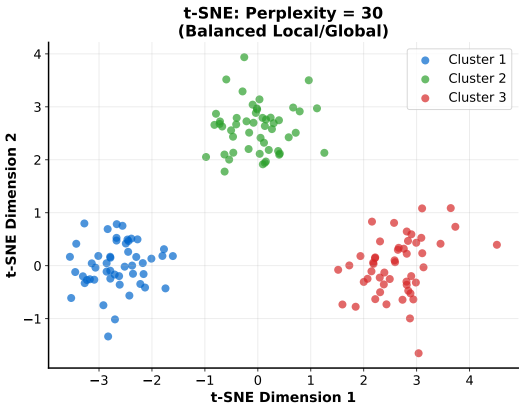
$$KL(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

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



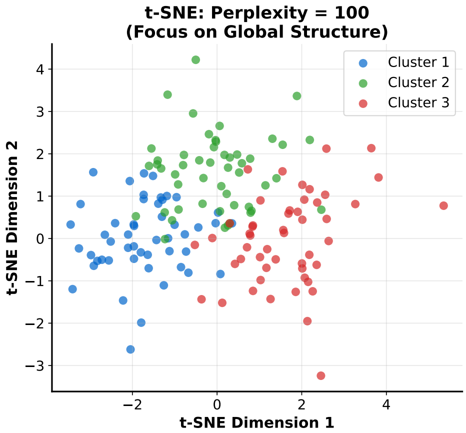
https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/04a_tsne_perplexity_5

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



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/04b_tsne_perplexity_30

Default perplexity (30): balanced local and global structure



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/04c_tsne_perplexity_100

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

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

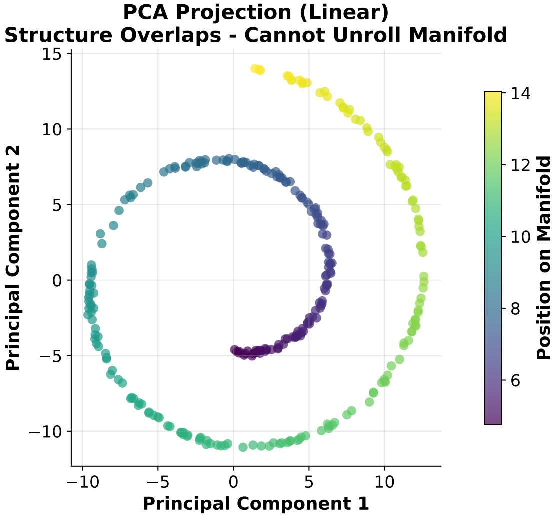
Important Limitations:

- 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:

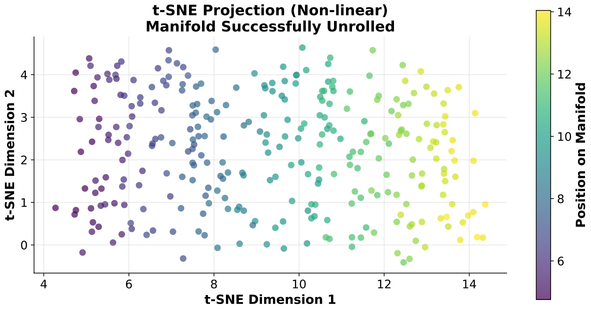
- Use PCA first to reduce to 30-50 dims
- Run multiple times with different seeds
- Don't over-interpret cluster sizes/distances
- Use for exploration, not final conclusions

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



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/05a_pca_swiss_roll

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

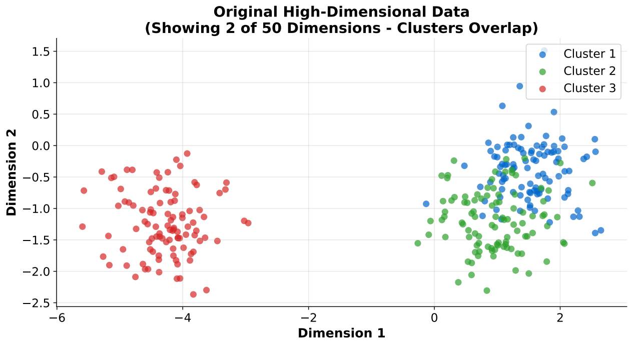


https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/05b_tsne_swiss_roll

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

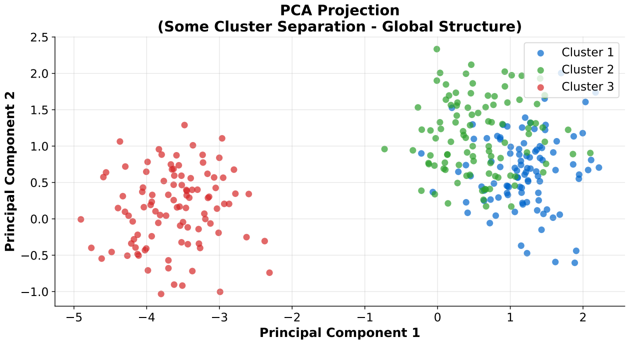
Aspect	**PCA**	**t-SNE**
Type	Linear	Non-linear
Speed	Fast $O(np^2)$	Slow $O(n^2)$
Deterministic	Yes	No
Preserves	Global variance	Local neighbors
Reversible	Yes	No
Use for ML	Yes (preprocessing)	No
Visualization	Okay	Excellent

Use PCA for preprocessing, t-SNE for visualization only



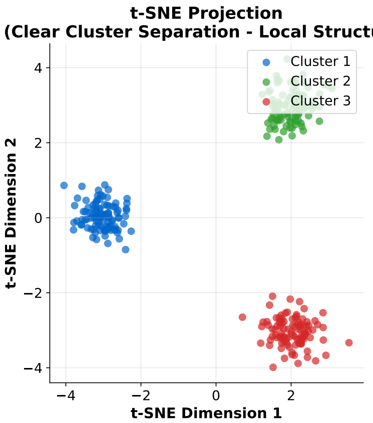
https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/06a_original_clusters

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



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/06b_pca_cluster_projection

PCA finds directions of max variance - some cluster separation



https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/06c_tsne_cluster_projection

t-SNE preserves local structure - clear cluster separation

Use PCA When:

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

Use t-SNE When:

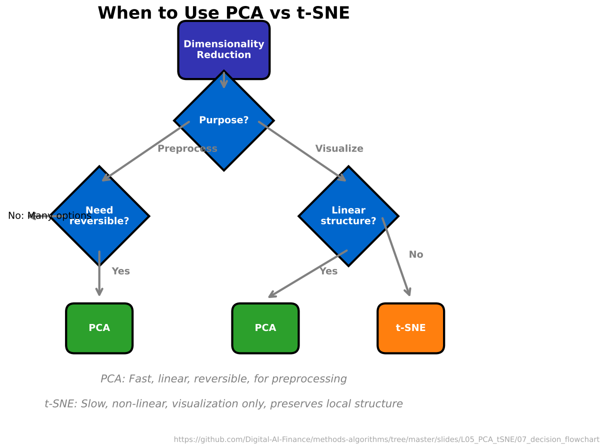
- Visualizing high-dimensional data
- Looking for cluster structure
- Non-linear manifolds expected
- Exploratory analysis

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

Open the Colab Notebook

- Exercise 1: Apply PCA to high-dimensional finance data
- Exercise 2: Visualize clusters with t-SNE
- Exercise 3: Compare PCA vs t-SNE for different datasets

Link: `https://colab.research.google.com/` [TBD]


When to Use PCA vs t-SNE
Dimensionality Reduction
Purpose?
Preprocess
Visualize
Need reversible?
Linear structure?
No: Many options
Yes
Yes
No
PCA
PCA
t-SNE
PCA: Fast, linear, reversible, for preprocessing
t-SNE: Slow, non-linear, visualization only, preserves local structure
https://github.com/Digital-AI-Finance/methods-algorithms/tree/master/slides/L05_PCA_tSNE/07_decision_flowchart

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

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

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

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

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