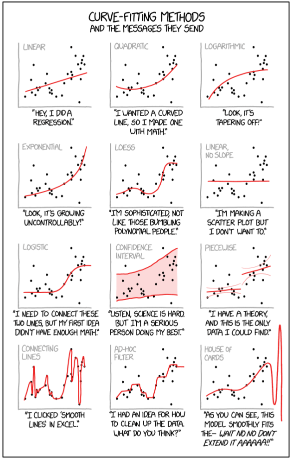
PCA & t-SNE

Mini-Lecture: Seeing the Big Picture in High Dimensions

Methods & Algorithms

MSc Data Science – Spring 2026

When You Have Too Many Dimensions to Plot

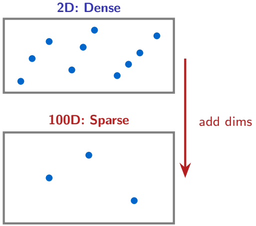


XKCD #2048 by Randall Munroe (CC BY-NC 2.5)

The Curse of Dimensionality

Why High-Dimensional Data Is Hard

- In high dimensions, all points become equally distant – nearest-neighbor methods break down
- A dataset that seems dense in 2D becomes sparse in 100D
- Visualization is impossible beyond 3 dimensions
- Many features are redundant or correlated – we need to compress without losing structure



Key Question

Can we reduce 100 features to 2–3 while preserving the important patterns?

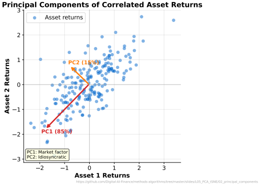
Bellman (1961) coined "curse of dimensionality" – the volume of space grows exponentially with dimensions

PCA: Find the Directions of Maximum Variance

Principal Component Analysis

- **Step 1**: Center the data (subtract the mean)
- **Step 2**: Find the direction of maximum variance – that is PC1
- **Step 3**: Find the next orthogonal direction of maximum variance – that is PC2
- Project data onto these new axes to reduce dimensions

Mathematically: eigendecomposition of the covariance matrix $\Sigma = \frac{1}{n} X^T X$.



Insight

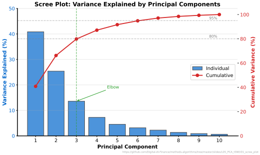
PCA is a rotation – it does not discard data, it reorders it by importance (variance).

PCA preserves global structure (variance) – it finds the best linear summary of your data

How Many Components Do We Keep?

The Scree Plot

- Plot explained variance ratio for each component
- Look for the "elbow" – where additional components add little
- Rule of thumb: keep enough components to explain 90–95% of total variance
- Alternatively, use cross-validation on a downstream task



Insight

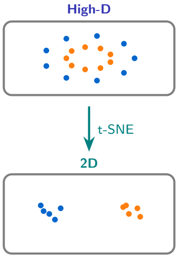
If 3 components explain 95% of variance in 50 features, you have compressed 50D to 3D with minimal information loss.

The scree plot is named after the geological term for rubble at the base of a cliff – you stop where the "cliff" flattens

t-SNE: Preserving Neighborhoods in 2D

When Linear Projection Fails

- t-SNE (van der Maaten & Hinton, 2008) is a non-linear method for visualization
- Converts high-D distances to probabilities, then matches them in 2D
- Preserves **local structure**: nearby points stay nearby
- Warning: global distances are not meaningful in t-SNE plots



Insight

t-SNE is for looking at your data, not for feeding into a model. Use PCA for preprocessing, t-SNE for visualization.

t-SNE clusters are real (local structure is preserved), but cluster distances and sizes are not – never interpret gaps

Perplexity: t-SNE's Key Hyperparameter

Balancing Local vs Global Structure

- **Perplexity** ≈ effective number of neighbors each point considers
- Low perplexity (5–10): tight local clusters, noisy global layout
- High perplexity (30–50): smoother layout, may merge distinct groups
- Always try multiple perplexity values before drawing conclusions

Perplexity	Behavior
5	Very local, fragmented clusters
30	Balanced (default in sklearn)
50	Smoother, global trends visible
100+	Over-smoothed, clusters merge

Rule of thumb: perplexity should be smaller than $n/3$ where n is the number of data points.

Insight

There is no "correct" perplexity. If your conclusions change with perplexity, they are artifacts of the method, not real structure.

Wattenberg et al. (2016) "How to Use t-SNE Effectively" – essential reading before interpreting t-SNE plots

PCA vs t-SNE: When to Use Which?

Comparison Table

Property	**PCA**	**t-SNE**
Type	Linear	Non-linear
Preserves	Global variance	Local neighborhoods
Invertible	Yes (reconstruct data)	No
Speed	Fast ($O(np^2)$)	Slow ($O(n^2)$)
Deterministic	Yes	No (random initialization)
Use for modeling	Yes (preprocessing)	No (visualization only)
Interpretable axes	Yes (loadings)	No

Practical Advice

Run PCA first to reduce to 30–50 dimensions, then apply t-SNE for visualization. This is faster and more stable than running t-SNE on raw high-D data.

PCA + t-SNE pipeline: PCA for compression and denoising, t-SNE for the final 2D visualization

Finance Application: Yield Curve PCA

The Three Factors of Interest Rates

- PCA on yield curve data (1Y, 2Y, 5Y, 10Y, 30Y rates) reveals 3 dominant components
- **PC1 (∼85%)**: Level – parallel shift of all rates
- **PC2 (∼10%)**: Slope – short vs long rates diverge
- **PC3 (∼3%)**: Curvature – belly of the curve moves

Insight

3 components explain 98% of yield curve variation. Fixed income risk management is built on this PCA decomposition.

Portfolio Risk with PCA:

Instead of tracking 10 maturities, track 3 factor exposures:

$$\Delta P \approx D_1 \cdot \Delta\text{PC1} + D_2 \cdot \Delta\text{PC2} + D_3 \cdot \Delta\text{PC3}$$

D_k: factor duration (sensitivity to factor k)

Litterman & Scheinkman (1991) showed that 3 PCA factors explain >98% of US Treasury yield curve movements

Summary: Dimensionality Reduction in 4 Takeaways

1. **Curse of dimensionality**: high-D data is sparse, distances become meaningless, and visualization is impossible without reduction
2. **PCA**: linear, fast, invertible – finds directions of maximum variance. Use for preprocessing and interpretable compression.
3. **t-SNE**: non-linear, slow, for visualization only – preserves local neighborhoods but not global distances. Always try multiple perplexity values.
4. **Finance**: yield curve PCA (level, slope, curvature) reduces 10+ maturities to 3 factors explaining 98% of variance

Next Steps

Explore the deep dive slides for eigenvalue derivations, kernel PCA, and UMAP. Try the Jupyter notebook to run PCA on real financial data.

PCA is a tool; t-SNE is a lens. Use PCA to simplify your data, use t-SNE to look at it.