Empirical Verification of the Variance–Reconstruction Error Equivalence in PCA

ECE 57000 AI Course Project – TinyReproductions Track • Anonymous submission

Motivation and Problem

- High-dimensional data (images, text, tabular features) are hard to visualize and reason about directly.
- Linear dimensionality reduction methods project data into a lower-dimensional subspace.
- Principal Component Analysis (PCA) is a classic method that chooses directions of maximum variance.
- A theoretical result says: for mean-centered data and fixed dimension k, PCA both
  - maximizes captured variance, and
  - minimizes squared reconstruction error
  among all rank-k linear projections.

Experimental Setup

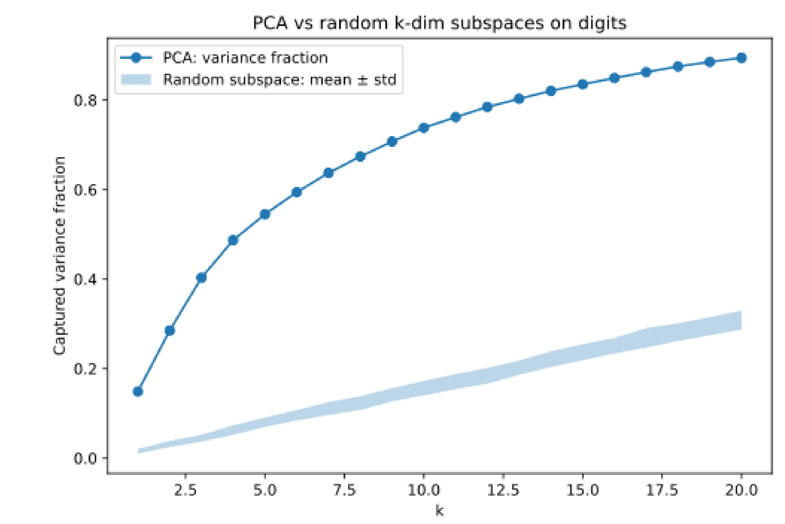
- Dataset: scikit-learn digits ($n \approx 1797$, $d = 64$).
- Preprocessing: mean-center each feature to obtain X_c.
- For each $k \in \{1,\ldots,20\}$:
  - PCA: fit PCA and keep top k components.
  - Random subspaces: sample Gaussian matrix, orthonormalize columns by QR to get a random k-dimensional subspace.
- Metrics:
  - captured variance fraction = variance of projection / total variance
  - reconstruction quality = 1 − (mean-squared reconstruction error / total baseline MSE)

Reference:
Kevin P. Murphy, "Machine Learning: A Probabilistic Perspective," MIT Press, 2012.

On the digits dataset, PCA captures more variance and achieves lower reconstruction error than random linear subspaces for every k

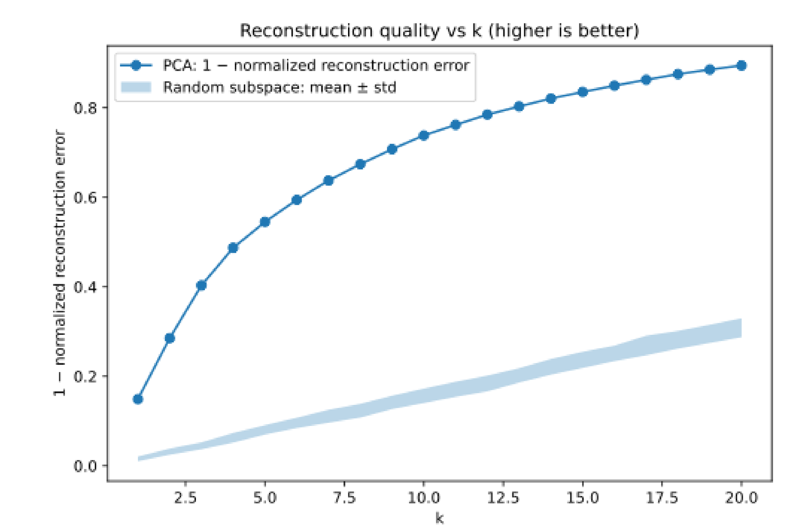
Results: Variance vs k

- Fraction of total variance captured vs k for PCA and random orthonormal k-dimensional subspaces.
- PCA curve lies above the random-subspace mean for all k = 1,…,20.
- The gap is largest for small k, where the choice of subspace matters most.
- As k increases, both PCA and random subspaces approach full variance, so curves converge.



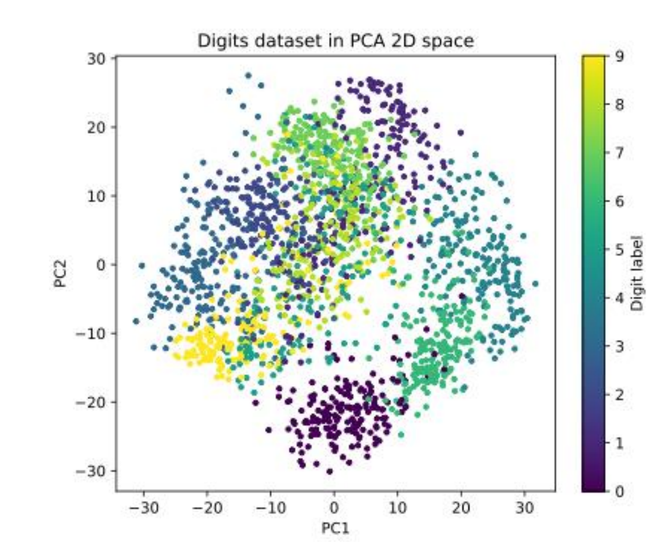
Results: Reconstruction Quality vs k

- Metric: reconstruction quality = 1 − normalized mean-squared error.
- PCA dominates the random baseline here as well for every k.
- Variance and reconstruction are complementary: capturing more variance means lower reconstruction error.



Visualization: 2D PCA Embedding

- Projection onto the first two principal components reveals clusters by digit label.
- Even in 2D, several digits form distinct regions, showing PCA finds meaningful structure.



Conclusion and Limitations

- This tiny reproduction empirically confirms that PCA is extremal for both variance and reconstruction error on the digits dataset.
- Limitations: single dataset ($d = 64$), only linear PCA, random isotropic baselines, in-sample evaluation.
- Future work: apply to other datasets, add train/test splits, compare with truncated SVD and nonlinear methods.