Unsupervised Dimensionality Reduction via PCA

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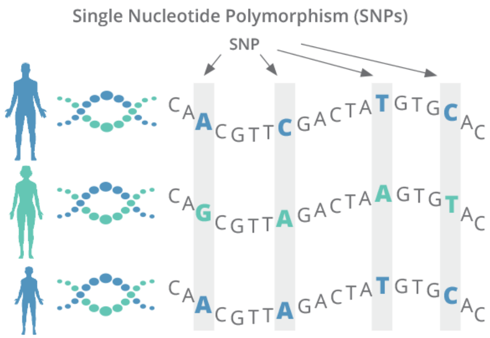
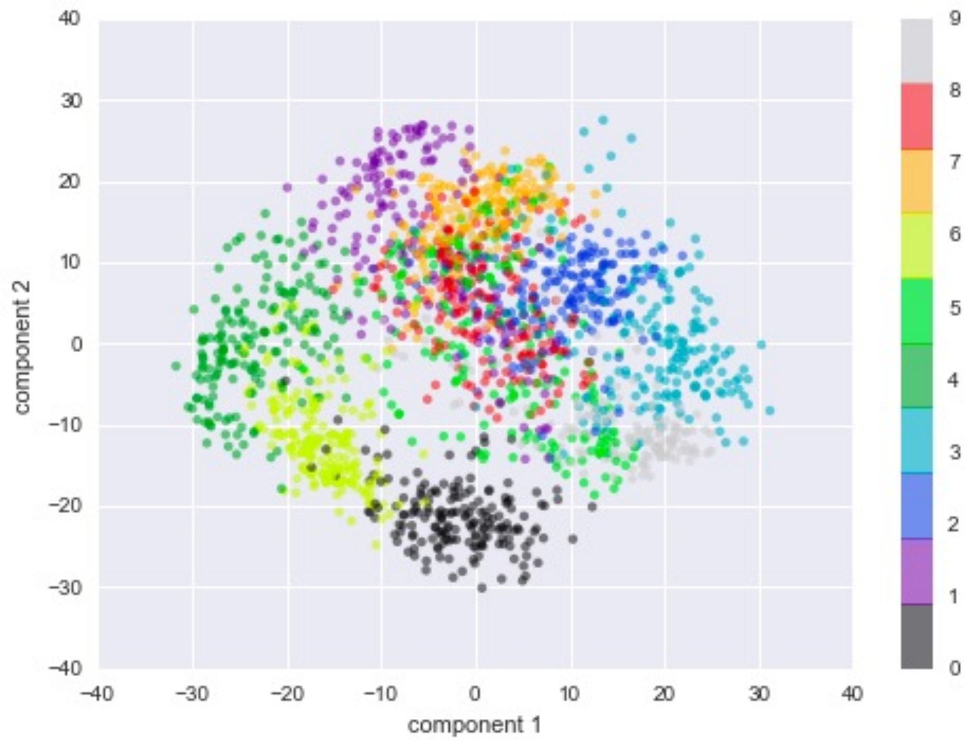
Very high-dimensional data is becoming ubiquitous



- Images (1 million pixels)
- Text (100k unique words)
- Genetics (4 million SNPs)
- Business data (12 million products)

Why dimensionality reduction? Visualization

- Allows 2D scatterplot visualizations even of high-dimensional data (2D projection of digits)

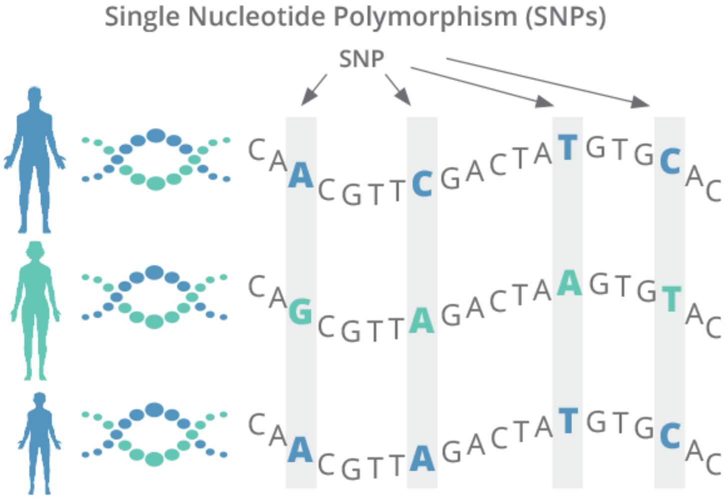


https://jakevdp.github.io/PythonDataScienceHandbook/05.09-principal-component-analysis.html

Why dimensionality reduction?
Lower computation costs

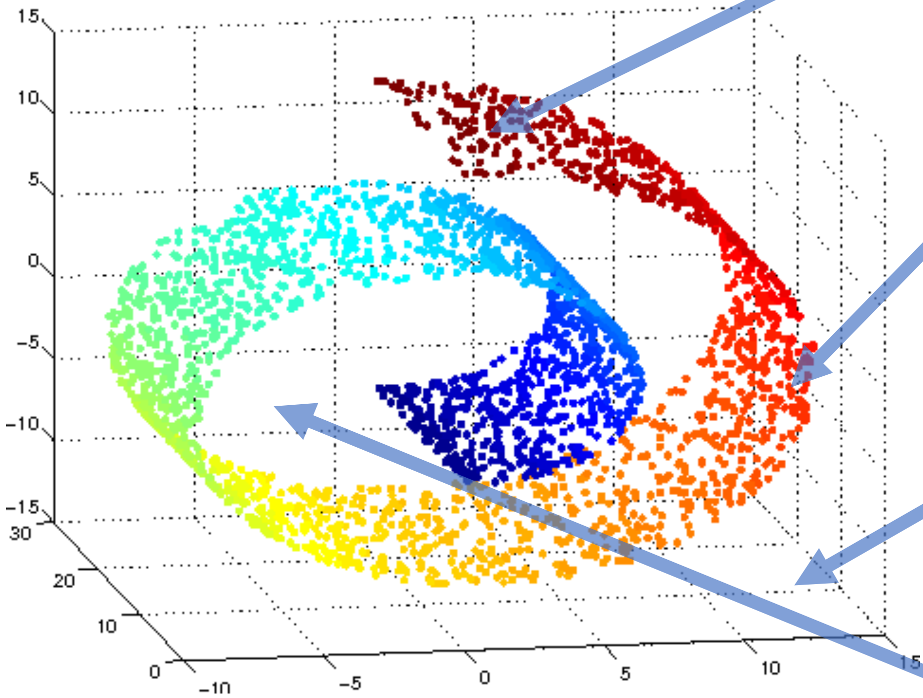
- Suppose original dimension is large like $\mathrm{d}=100000$ (e.g., images, DNA sequencing, or text)

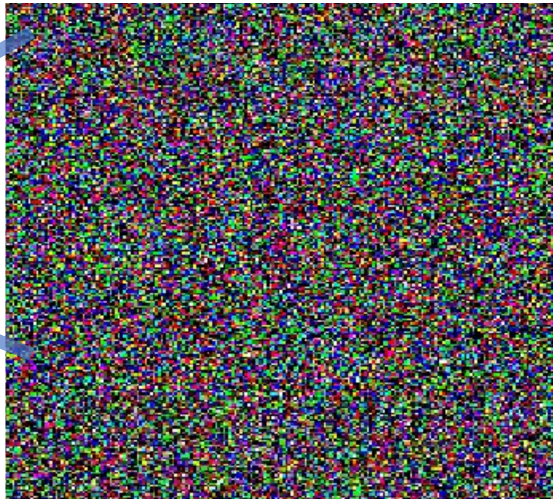
- If we reduce to $k=100$ dimensions, the training algorithm can be sped up by $1000\times$



4-5 million SNPs in human genome.
https://www.diagnosticsolutionslab.com/tests/genomicinsight

Why dimensionality reduction?
Underlying phenomena is on lower dimensional space





Outline of Principal Components Analysis (PCA)

1. Motivation for dimensionality reduction
2. Formal PCA problem: Min reconstruction
3. Derive PCA formulation for 1D
   - Least error 1D projection is orthogonal
   - Sum over all data points
4. Solution is based on truncated SVD
5. Equivalent problem: Max variance

Math: Principal Component Analysis (PCA) can be formalized as minimizing the *linear* reconstruction error of the data using only $k \le d$ dimensions

- PCA can be formalized as

$$\min_{Z \in \mathbb{R}^{n \times k}, W \in \mathbb{R}^{d \times k}} \|X_c - ZW^T\|_F^2 \quad \text{s.t. } W^T W = I_k$$

  - where

$$\mathrm{X_c} = \mathrm{X} - \mathbf{1}_n \mu_x^T \in \mathbb{R}^{n \times d} \quad \text{(centered input data)}$$

Review of linear algebra and introduction to numpy Python library

- See Jupyter notebook, which can be opened and run in Google Colab

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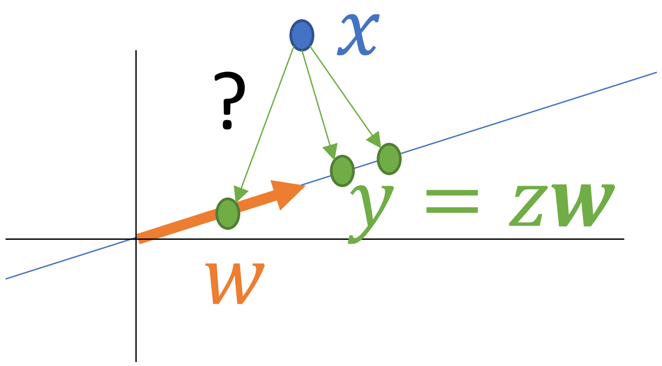
Math: Principal Component Analysis (PCA) can be formalized as minimizing the linear reconstruction error of the data using only $k \leq d$ dimensions

$$\min_{Z \in \mathbb{R}^{n \times k}, W \in \mathbb{R}^{d \times k}} \|X_c - ZW^T\|_F^2 \;\; \text{s.t. } W^T W = I_k$$

- Let's stare at this equation some more ☺
- What does the orthogonal constraint mean?
- Why minimize the squared Frobenius norm?
- $\|X_c - ZW^T\|_F^2 = \sum_{i=1}^n \left\|\boldsymbol{x}_i^T - \boldsymbol{z}_i^T W^T\right\|_2^2 = \sum_{i=1}^n \|\boldsymbol{x}_i - W \boldsymbol{z}_i\|_2^2$
- For analysis, let's simplify to a single dimension (i.e., $k = 1$)
  - $\sum_{i=1}^n \|\boldsymbol{x}_i - z_i \boldsymbol{w}\|_2^2$ where z_i is a scalar

What is the best projection given a fixed subspace (line in 1D case)?

- If we are given $\boldsymbol{w}$, what is the best z (i.e. minimum reconstruction error) for a given $\boldsymbol{x}$?
  - $\min_z \|\boldsymbol{x} - z\boldsymbol{w}\|_2^2$



- The orthogonal projection!
  - $z = \boldsymbol{x}^T\boldsymbol{w} = \|\boldsymbol{x}\|\|\boldsymbol{w}\|\cos\theta = \|\boldsymbol{x}\|\cos\theta$
  - $z = \|\boldsymbol{x}\|\cos\theta = \text{hyp}\cdot\frac{\text{adj}}{\text{hyp}} = \text{adj}$
  - $z\boldsymbol{w}$ is a scaled vector along the line defined by $\boldsymbol{w}$

Thus, we can simplify to only minimizing over W

$$\min_{\boldsymbol{z},\boldsymbol{w}:\|\boldsymbol{w}\|_2=1} \sum_{i=1}^{n} \|\boldsymbol{x_i} - z_i \boldsymbol{w}\|_2^2 = \min_{\boldsymbol{w}:\|\boldsymbol{w}\|_2=1} \sum_{i=1}^{n} \left\|\boldsymbol{x_i} - \left(\boldsymbol{x}_i^T \boldsymbol{w}\right)\boldsymbol{w}\right\|_2^2$$

- Now we can return to the Frobenius norm:

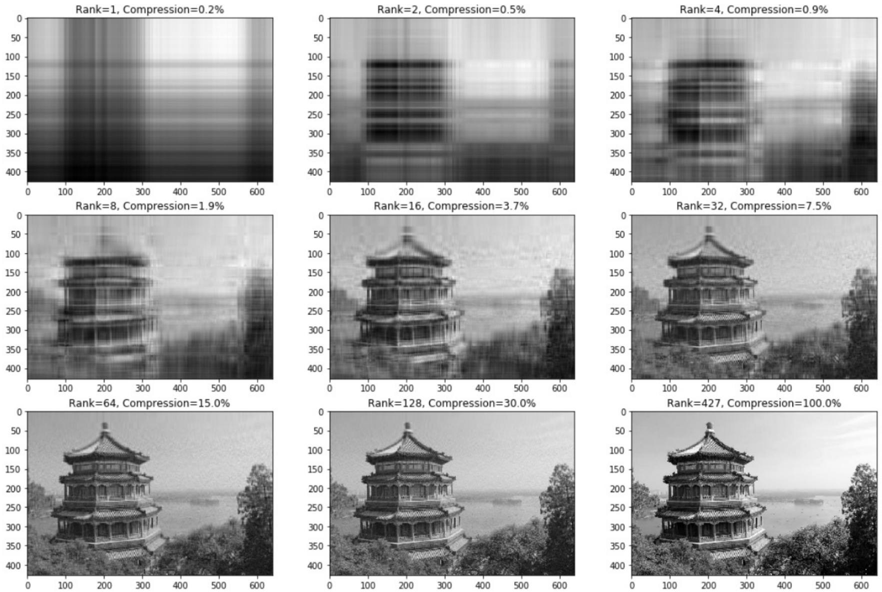
$$\min_{\boldsymbol{w}:\|\boldsymbol{w}\|_2=1} \left\|X_c - \boldsymbol{z}\boldsymbol{w}^{\boldsymbol{T}}\right\|_F^2 \quad \text{where} \quad \boldsymbol{z} = X_c \boldsymbol{w}$$

- What is $\boldsymbol{z}\boldsymbol{w}^{\boldsymbol{T}}$? Have we seen something like this before?
- This is the best rank-1 approximation to X_c, which is given by the SVD!
  - $\boldsymbol{w} = \boldsymbol{v}_1$ and $\boldsymbol{z} = \sigma_1 \boldsymbol{u}_1$, where $\sigma_1, \boldsymbol{u}_1, \boldsymbol{v}_1$ are the first singular value, left singular vector and right singular vector respectively.

For $k \geq 1$, the PCA solution is the top k right singular vectors

- If $X_c = USV^T$, then the general solution is
$$W^* = V_{1:k}$$

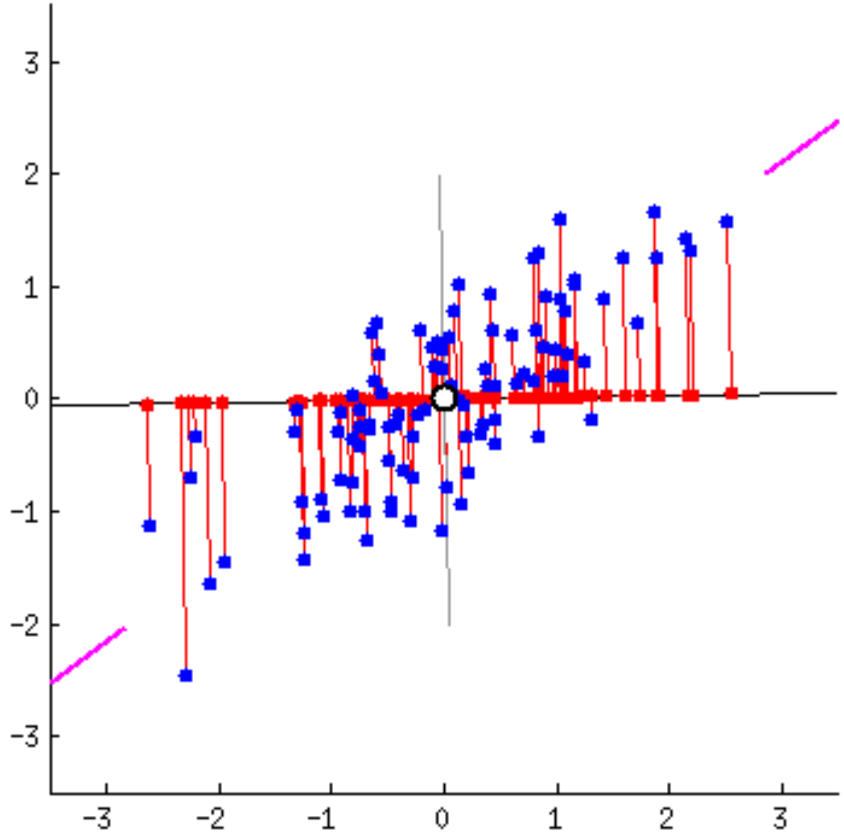
- Remember: SVD is best k dim. approximation



Intuition: Principal component analysis finds the **best linear projection** onto a lower-dimensional space

$$\min_{\boldsymbol{w}:\|\boldsymbol{w}\|_2=1} \left\| X_c - \boldsymbol{z}\boldsymbol{w}^{\boldsymbol{T}} \right\|_F^2$$

where $\boldsymbol{z} = X_c \boldsymbol{w}$



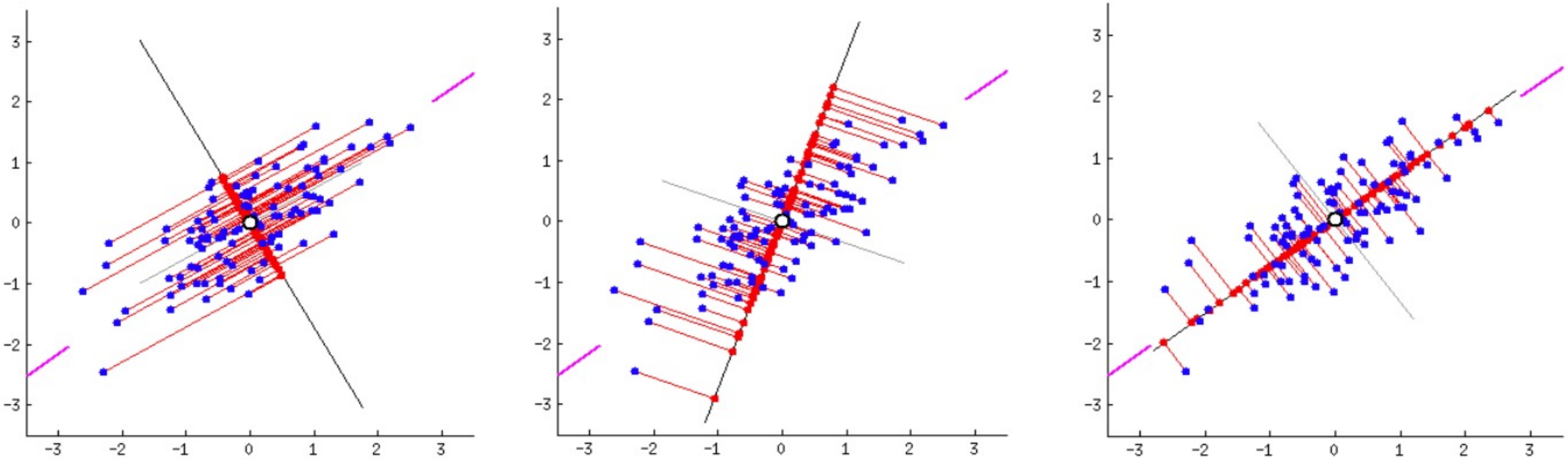
2D to 1D projection: Red lines show the projection error onto 1D lines. PCA finds the line that has the smallest projection error (in this example, when it aligns with the purple).

https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues

Minimizing reconstruction error (red lines) is equivalent to maximizing the variance of projection (spread of red points)

Max reconstruction error
Min variance

Min reconstruction error
Max variance



$$\underset{\boldsymbol{w}:\|\boldsymbol{w}\|_2=1}{\operatorname{argmin}} \left\| X_c - \boldsymbol{z}\boldsymbol{w}^T \right\|_F^2$$

$$= \underset{\boldsymbol{w}:\|\boldsymbol{w}\|_2=1}{\operatorname{argmax}} \sigma_z^2$$

where $\boldsymbol{z} = X_c \boldsymbol{w}$

Derivation of equivalence will require 2 facts

1. The squared Frobenius norm is equal to the trace of matrix times itself:
   - $||A||_F^2 = \mathrm{Tr}(A^T A) = \mathrm{Tr}(A A^T)$
2. Optimization solutions are invariant when the objective is multiplied by **positive** constant or a constant is added,
   - $\underset{W}{\operatorname{argmin}} f(W) = \underset{W}{\operatorname{argmin}} a f(W) + b, \quad \forall a > 0, b \in \mathbb{R}$

The PCA objective can be decomposed into the original variance minus the variance of projection

- Minimize reconstruction error
$$\min_{W:W^TW=I_k} \|X_c - ZW^T\|_F^2, \qquad \text{where } Z = X_cW$$
- $\|X_c - ZW^T\|_F^2$
- $= \mathrm{Tr}\big((X_c - ZW^T)(X_c - ZW^T)^T\big)$
- $= \mathrm{Tr}(X_cX_c^T - 2ZW^TX_c^T + ZW^T(ZW^T)^T)$
- $= \mathrm{Tr}(X_cX_c^T - 2ZZ^T + ZW^TWZ^T)$
- $= \mathrm{Tr}(X_cX_c^T - 2ZZ^T + ZZ^T)$
- $= \mathrm{Tr}(X_cX_c^T - ZZ^T)$
- $= \mathrm{Tr}(X_cX_c^T) - \mathrm{Tr}(ZZ^T)$
- $= \mathrm{Tr}(X_c^TX_c) - \mathrm{Tr}(Z^TZ)$

Equivalence is derived by manipulating optimization problem

- $\underset{W:W^TW=I_k}{\operatorname{argmin}} \|X_c - (X_cW)W^T\|_F^2$
- $= \underset{W:W^TW=I_k}{\operatorname{argmin}} \operatorname{Tr}[X_c^T X_c] - \operatorname{Tr}[Z^T Z]$
- $= \underset{W:W^TW=I_k}{\operatorname{argmin}} -\operatorname{Tr}[Z^T Z]$
- $= \underset{W:W^TW=I_k}{\operatorname{argmax}} \operatorname{Tr}[Z^T Z]$
- $= \underset{W:W^TW=I_k}{\operatorname{argmax}} \sum_{j=1}^{k} \hat{\sigma}_{z,j}^2$

(sum of variances in projected space)

Equivalent solutions: The solution to both problems is the top k right singular vectors of X_c

- Minimize reconstruction error
$$\min_{W:W^TW=I_k} \|X_c - (X_cW)W^T\|_F^2$$
  - Singular value decomposition (SVD) of $X_c = USV^T$
  - Solution: $W^* = V_{1:k}$

- Maximize variance of latent projection (equivalent solution)
$$\max_{W:W^TW=I_k} \mathrm{Tr}(Z^TZ) = \sum_{j=1}^{k} \hat{\sigma}_{Z,j}^2$$
  - Equivalent solution is the eigenvectors of $X_c^TX_c = n\hat{\Sigma}$
    - $X_c^TX_c = (USV^T)^T(USV^T) = (VSU^T)(USV^T) = VS(U^TU)SV^T = VS^2V^T = Q\Lambda Q^T$
  - Solution: $W^* = Q_{1:k} \equiv V_{1:k}$!

Recap: Principal Components Analysis (PCA)

1. Motivation for dimensionality reduction
2. Formal PCA problem: Min reconstruction
3. Derive PCA formulation for 1D
   - Least error 1D projection is orthogonal
   - Sum over all data points
4. Solution is based on truncated SVD
5. Alternative viewpoint: Max variance
   - Derive equivalence
   - Derive equivalent solutions

Demo of PCA via sklearn (time permitting)

- Random projections vs PCA projections
- Visualizations of
  - Minimum reconstruction error
  - Maximum variance
  - Explained variance based on k
- Code examples
  - Digits
  - Eigenfaces

Questions?