Dimensionality Reduction

We want to represent data in a new coordinate system with fewer dimensions, while preserving as much *information* as possible

Why?

- Can't easily visualize high dimensional data, but can easily plot 2D (and 3D data)
- We want to extract features from the data (e.g. to build a linear regression model)
- We want to compress the data while preserving most of the information

Preserving Information

What does it mean to preserve *as much information* as possible?

- Preserve **distance** between data points
- Preserve **variations** in the data

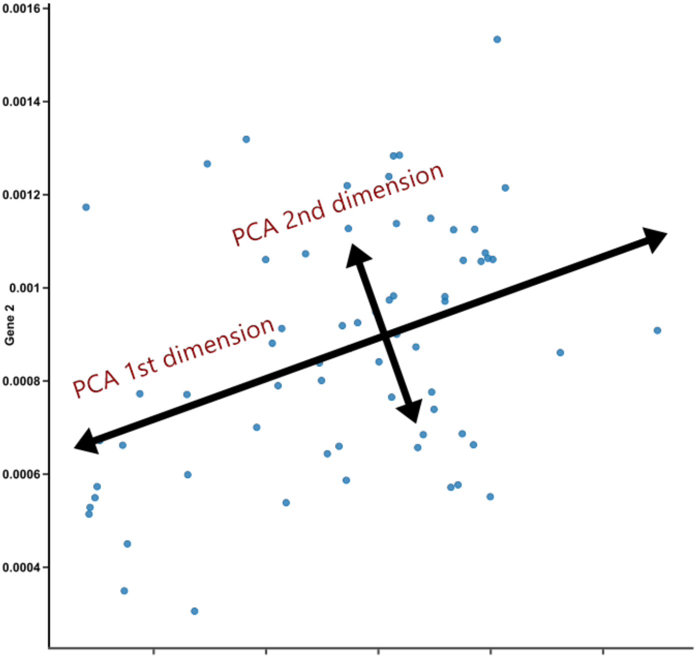
Principal Component Analysis

PCA is a **linear** dimensionality reduction technique

The transformed data is a linear transformation of the original data

We want to find a hyperplane that the data lies in and project the data onto that hyperplane

PCA 2D to 1D

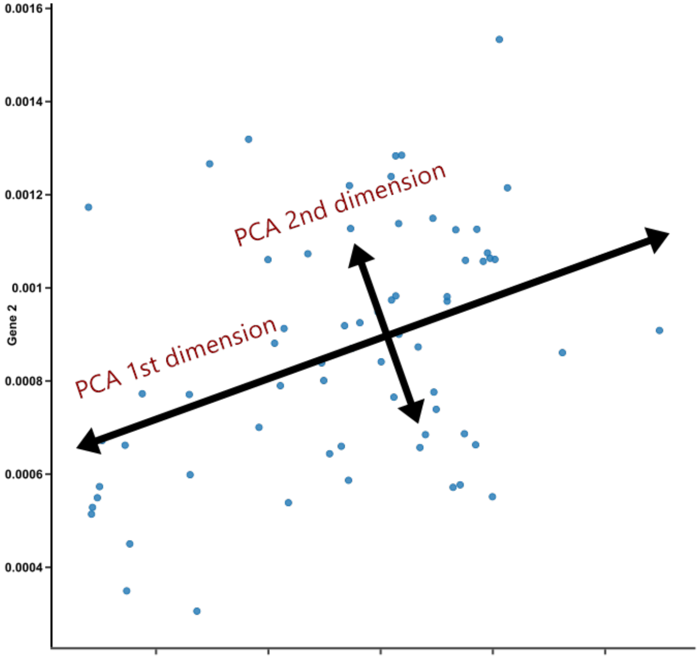


0.0016
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
Gene 2
PCA 2nd dimension
PCA 1st dimension

PCA: Key Idea

1. **Rotate** the data with some rotation matrix R so that the new features are uncorrelated
2. **Keep** only the dimensions with the **highest variance** (same as preserving distance)

PCA Rotation Picture



PCA Derivation

We want to identify directions in our data dimension with high variance

Let A be our data, where A is $m \times n$, and A is normalized (so the mean of each column of A is zero)

Look at the covariance matrix $E = A^T A$. The spectral theorem says that we can diagonalize E:

$$E = RDR^T$$

Where D is diagonal and R is orthogonal. The diagonals of D are the eigenvalues. The columns of R are eigenvectors of E.

Do you remember what eigenvectors are?

Why PCA

$$
\begin{aligned}
E &= RDR^T \\
A^T A &= R^T DR \\
R^T A^T AR &= D \\
(RA)^T (AR) &= D
\end{aligned}
$$

So if we rotate A using R, the covariance of the transformed data will be diagonal.

The columns of AR is uncorrelated.

Numerical Problem

Given $E = A^T A$, find orthogonal R, diagonal D such that

$$E = RDR^T$$

Finding one eigenvector/eigenvalues

Finding the largest eigenvalue and the corresponding eigenvector is straightforward using **Power Iteration**.

Start with a random vector $\mathbf{x}$ in $\mathbb{R}^n$, and repeatedly compute

$$\mathbf{x} = A\mathbf{x}$$

(Does this remind you of fixed-point iteration?)

Finding one eigenvector/eigenvalues

Note: the norm of $\mathbf{x}$ might grow, so normalize instead

$$\mathbf{x} = A\mathbf{x}$$
$$\mathbf{x} = \frac{\mathbf{x}}{||\mathbf{x}||}$$

Finding many eigenvectors/eigenvalues

In linear algebra class, you might have used the characteristic polynomial

In numerical computing, we use *simnultaneous iteration*: similar idea to *power iteration*, but we try to find multiple eigenvectors/eigenvalues at the same time! Use a matrix X instead of $\mathbf{x}$

We need to make sure that we find different eigenvectors/eigenvalues, so we want the columns of X to be orthogonal!

Compute QR factorization of X in each iteration

Finding many eigenvectors/eigenvalues

In each iteration:

- Compute the QR factorization of X
- Replace X with AQ

We can find *all* the eigenvectors/eigenvalues in the same way.

(We'll skip the discussion on sensitivity and conditioning. Generally, the problem becomes ill-conditioned when you have eigenvalues that are close to each other)

Singular Value Decomposition

Instead of computing the eigenvalue decomposition of $A^T A$, computing the **singular value decomposition** of A is a better conditioned problem.

$A = U \Sigma V^T$

Where U is $m \times m$ and orthogonal, V is $n \times n$ and orthogonal, and Σ is $m \times n$ and diagonal.

The diagonal entries of Σ are called *singular values*

SVD vs Eigendecomposition

The eigenvalues of $A^T A$ are squares of the singular values of A. If we have the SVD of $A = U\Sigma V^T$ then

$$\begin{aligned} A^T A &= (U\Sigma V^T)^T (U\Sigma V^T) \\ &= V\Sigma^T U^T U\Sigma V^T \\ &= V\Sigma^T \Sigma V^T \end{aligned}$$

Which gives us the eigenvalue decomposition $A^T A = RDR^T$

SVD and QR Decomposition

QR Decomposition:

$$A = Q \begin{bmatrix} R \\ O \end{bmatrix}$$

Where Q is $m \times m$ and orthogonal, F is $n \times n$ and upper triangular.

Singular Value Decomposition:

$$A = U \Sigma V^T$$

Where U is $m \times m$ and orthogonal, V is $n \times n$ and orthogonal, and Σ is $m \times n$ and diagonal.