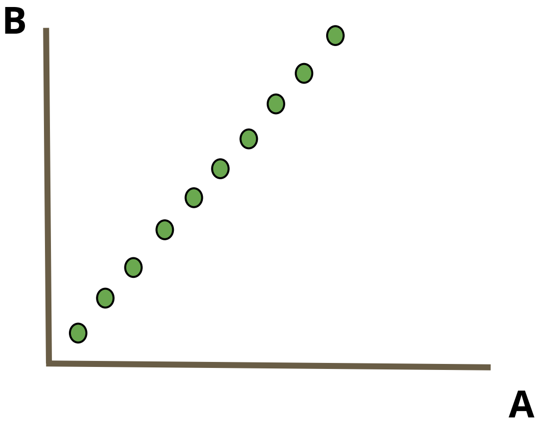
Singular Value Decomposition

Boston University CS 506 - Lance Galletti

Characteristics of a dataset to look for



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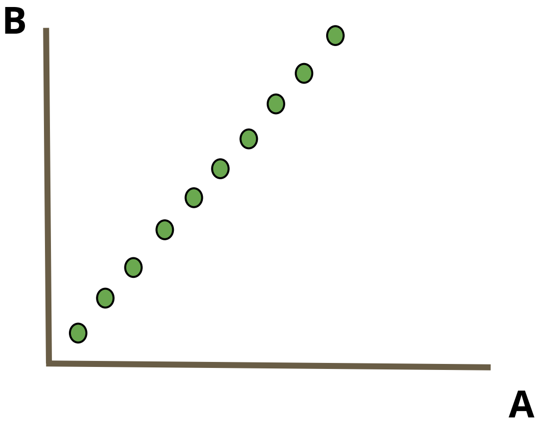

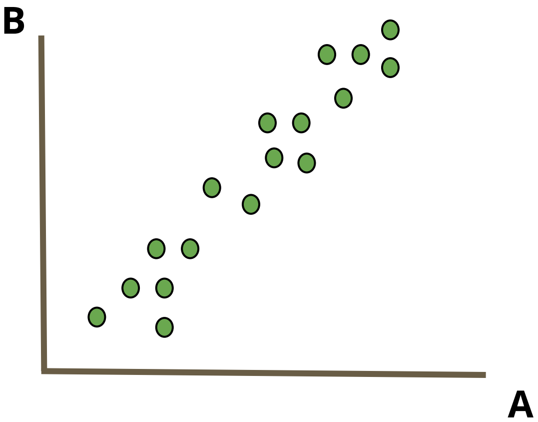

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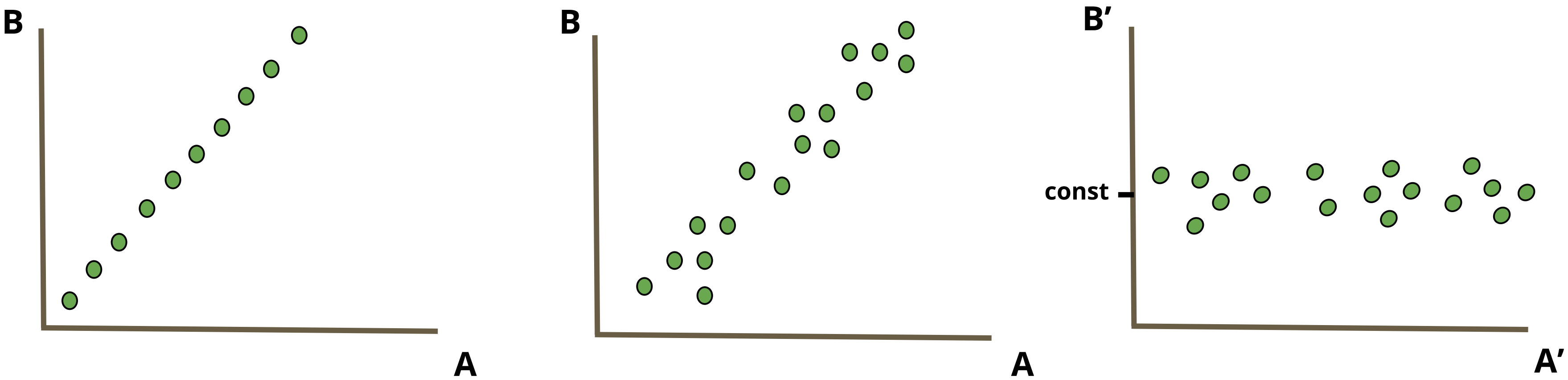

no relationship between A' and B'
(A' and B' are indepent)

$$
\text{\textbf{n} data points}\left\{
\begin{pmatrix}
x_{11} & \cdots & x_{1j} & \cdots & x_{1m} \\
\vdots & \ddots & \vdots & & \vdots \\
x_{i1} & \cdots & x_{ij} & \cdots & x_{im} \\
\vdots & & \vdots & \ddots & \vdots \\
x_{n1} & \cdots & x_{nj} & \cdots & x_{nm}
\end{pmatrix}\right.
$$

$$
\underbrace{\hphantom{x_{11} \quad \cdots \quad x_{1j} \quad \cdots \quad x_{1m}}}_{\textbf{m}\text{ features}}
$$

Goal

Examine this matrix and uncover its linear algebraic properties to:

1. Approximate A with a smaller matrix B that is easier to store but contains similar information as A

$$\begin{array}{cc}
 & \begin{array}{ccccc} \mathbf{A} & \ldots & \mathbf{J} & \ldots & \mathbf{M} \end{array} \\
\begin{array}{l} \textbf{n}\text{ data} \\ \text{points} \end{array} & \left\{ \underbrace{\begin{pmatrix}
x_{11} & \cdots & x_{1j} & \cdots & x_{1m} \\
\vdots & \ddots & \vdots & & \vdots \\
x_{i1} & \cdots & x_{ij} & \cdots & x_{im} \\
\vdots & & \vdots & \ddots & \vdots \\
x_{n1} & \cdots & x_{nj} & \cdots & x_{nm}
\end{pmatrix}}_{\textbf{m}\text{ features}} \right.
\end{array}
\qquad
\begin{array}{c}
\begin{array}{ccccc} \mathbf{A'} & \ldots & \mathbf{J'} & \ldots & \mathbf{M'} \end{array} \\
\underbrace{\begin{pmatrix}
x_{11} & \cdots & x_{1j} & \cdots & x_{1m} \\
\vdots & \ddots & \vdots & & \vdots \\
x_{i1} & \cdots & x_{ij} & \cdots & x_{im} \\
\vdots & & \vdots & \ddots & \vdots \\
x_{n1} & \cdots & x_{nj} & \cdots & x_{nm}
\end{pmatrix}}_{\textbf{m}\text{ features}}
\end{array}$$

Goal

Examine this matrix and uncover its linear algebraic properties to:

1. Approximate A with a smaller matrix B that is easier to store but contains similar information as A
2. Dimensionality Reduction / Feature Extraction

$$\begin{array}{cc} & \begin{array}{ccccc} \mathbf{A} & \ldots & \mathbf{J} & \ldots & \mathbf{M} \end{array} \\ \textbf{n}\text{ data points} \left\{ \vphantom{\begin{pmatrix} x \\ \vdots \\ x \\ \vdots \\ x \end{pmatrix}} \right. & \underbrace{\begin{pmatrix} x_{11} & \cdots & x_{1j} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots & & \vdots \\ x_{i1} & \cdots & x_{ij} & \cdots & x_{im} \\ \vdots & & \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nj} & \cdots & x_{nm} \end{pmatrix}}_{\textbf{m}\text{ features}} \end{array}$$

$$\begin{array}{c} \begin{array}{ccc} \mathbf{A''} & \ldots & \mathbf{J''} \end{array} \\ \underbrace{\begin{pmatrix} x_{11} & \cdots & x_{1j} \\ \vdots & \ddots & \vdots \\ x_{i1} & \cdots & x_{ij} \\ \vdots & & \vdots \\ x_{n1} & \cdots & x_{nj} \end{pmatrix}}_{\textbf{j}\text{ features}} \end{array}$$

Goal

Examine this matrix and uncover its linear algebraic properties to:

1. Approximate A with a smaller matrix B that is easier to store but contains similar information as A
2. Dimensionality Reduction / Feature Extraction
3. Anomaly Detection & Denoising

$$\begin{array}{c} \textbf{n}\text{ data} \\ \text{points} \end{array} \left\{ \underbrace{\begin{pmatrix} x_{11} & \cdots & x_{1j} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots & & \vdots \\ x_{i1} & \cdots & x_{ij} & \cdots & x_{im} \\ \vdots & & \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nj} & \cdots & x_{nm} \end{pmatrix}}_{\textbf{m}\text{ features}} \right.$$

Linear Algebra Review

Definition: The vectors in a set $\mathbf{V} = \{\vec{v}_1, \ldots, \vec{v}_n\}$ are **linearly independent** if

$$a_1\vec{v}_1 + \ldots + a_n\vec{v}_n = \vec{0}$$

can only be satisfied by $a_i = 0$

Note: this means no vector in that set can be expressed as a **linear combination** of other vectors in the set.

Linear Algebra Review

Definition:

The **determinant** of a square matrix A is a scalar value that encodes properties about the **linear mapping** described by A.

2x2:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

det(A) = ad - bc

Linear Algebra Review

Definition:

The **determinant** of a square matrix A is a scalar value that encodes properties about the **linear mapping** described by A.

3x3:

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \quad det(A) = a \cdot det\left(\begin{smallmatrix} e & f \\ h & i \end{smallmatrix}\right) - b \cdot det\left(\begin{smallmatrix} d & f \\ g & i \end{smallmatrix}\right) + c \cdot det\left(\begin{smallmatrix} d & e \\ g & h \end{smallmatrix}\right)$$

Linear Algebra Review

Definition:

The **determinant** of a square matrix A is a scalar value that encodes properties about the **linear mapping** described by A.

n X n:

Can recursively compute it. How?

Linear Algebra Review

Property:

n vectors $\{\vec{v}_1, \ldots, \vec{v}_n\}$ in an n-dimensional space are **linearly independent** iff the matrix **A**:

$$A = [\vec{v}_1, \ldots, \vec{v}_n] \quad (n \times n)$$

has non-zero determinant.

Q: Can **m > n** vectors in an **n**-dimensional space be linearly independent?

Linear Algebra Review

Definition:

The **rank** of a matrix **A** is the dimension of the vector space spanned by its column space. This is equivalent to the maximal number of linearly independent columns / rows of **A**.

Definition:

A matrix **A** is **full-rank** iff **rank(A) = min(m, n)**

Note: Get the rank of a matrix through the **Gram-Schmidt process**

Matrix Factorization

Any matrix **A** of rank **k** can be factored as

$$\mathbf{A} = \mathbf{U}\mathbf{V}$$

where

U is **n x k**
V is **k x m**

Matrix Factorization

To store an **n x m** matrix **A** requires storing **m · n** values.

However, if the rank of the matrix of **A** is **k**, since **A** can be factored as

$$\mathbf{A = UV}$$

which requires storing **k(m + n)** values.

In Practice

Most datasets are full rank despite containing a lot of redundant /similar information...

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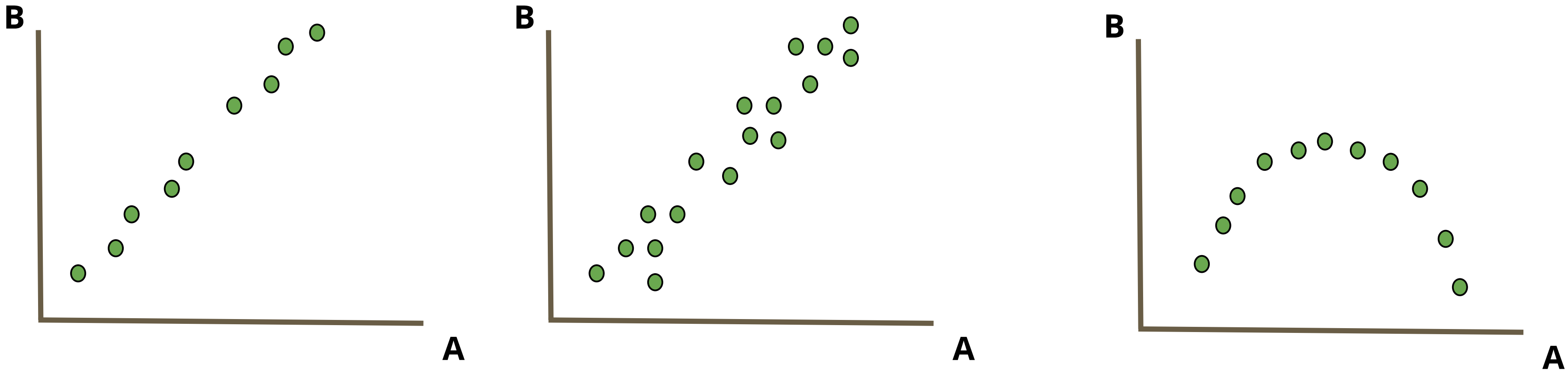


In Practice

Most datasets are full rank despite containing a lot of redundant /similar information...

But we might be able to approximate the dataset with a lower rank one that contains similar information.

Approximation

Goal:

Approximate **A** with $\mathbf{A}^{(k)}$ (low-rank matrix) such that

1. **d(A,** $\mathbf{A}^{(k)}$**)** is small
2. **k** is small compared to **m** & **n**

Frobenius Distance

$$d_F(A, B) = ||A - B||_F = \sqrt{\sum_{i,j} (a_{ij} - b_{ij})^2}$$

i.e. the pairwise sum of squares difference in values of A and B

Approximation

Definition:

When **k < rank(A)**, the **rank-k approximation** of **A** (in the least squares sense) is

$$A^{(k)} = \underset{\{B|rank(B)=k\}}{\arg\min} \; d_F(A, B)$$

Matrix Factorization Improved

Not only can we factorize a matrix **A** of rank **k** as **A = UV**. But we can factorize **A** using a process called Singular Value Decomposition where:

$$\mathbf{A} = \mathbf{U \Sigma V^T}$$

Approximation

Definition:

The **Singular Value Decomposition** of a rank-r matrix A has the form

$$\mathbf{A = U\Sigma V^T}$$

where

U is **n x r**
The **columns** of **U** are orthogonal & unit length (**$U^TU = I$**)

V is **m x r**
The **columns** of **V** are orthogonal & unit length (**$V^TV = I$**)

Approximation

Definition:

The **Singular Value Decomposition** of a rank-r matrix A has the form

$$\mathbf{A = U\Sigma V^T}$$

where

$$\Sigma = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{pmatrix}$$

with $\boldsymbol{\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0}$

$\boldsymbol{\sigma_i}$ is the square root of the eigenvalues of $\mathbf{A^TA}$ and are called **singular values**

Approximation

Find $\mathbf{A}^{(k)}$ by decomposing **A**:

$$A = \begin{pmatrix} \boxed{U_1} & U_2 \end{pmatrix} \begin{pmatrix} \boxed{\Sigma_1} & \\ & \Sigma_2 \end{pmatrix} \begin{pmatrix} \boxed{V_1} & V_2 \end{pmatrix}$$

$\mathbf{A}^{(k)} = \mathbf{U_1 \Sigma_1 V_1^T}$

Where

$\mathbf{U_1}$ is **n x k**
$\mathbf{\Sigma_1}$ is **k x k**
$\mathbf{V_1}$ is **m x k**

Approximation

1	1	1	0	0
2	2	2	0	0
1	1	1	0	0
5	5	5	0	0
0	0	0	2	2
0	0	0	3	3
0	0	0	1	1

=

0.18	0
0.36	0
0.18	0
0.90	0
0	0.53
0	0.80
0	0.27

x

9.64	0
0	5.29

x

0.58	0.58	0.58	0	0
0	0	0	0.71	0.71

Approximation

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

Approximation

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

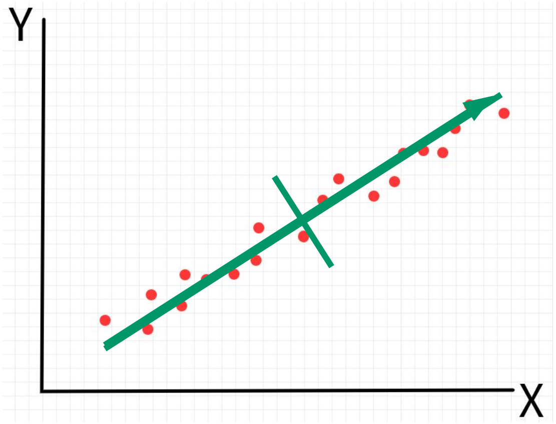
Approximation

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Approximation

The i^{th} **singular vector** represents the direction of the i^{th} most variance.

$$\Sigma = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{pmatrix}$$



Singular Values express the importance / significance of a singular vector

Approximation

Property:

$$d_F(A, A^{(k)})^2 = \sum_{i=k+1}^{r} \sigma_i^2$$

Note: the larger **k** is, the smaller the distance.

Approximation

To find the right **k** you can:

1. Look at the singular value plot to find the elbow point
2. Look at the residual error of choosing different **k**

Related to Principal Component Analysis (PCA)

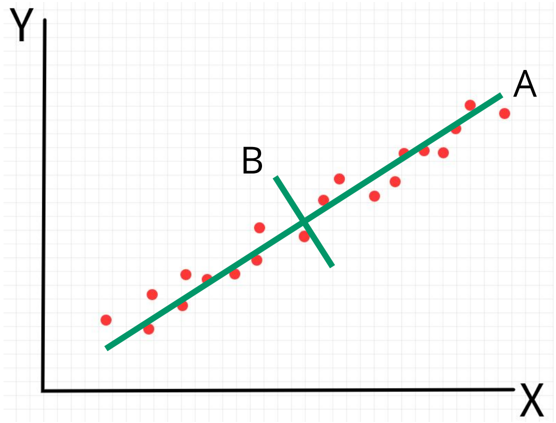
SVD and PCA are related

See demo

Dimensionality Reduction

Idea: project the data onto a subspace generated from a subset of singular vectors / principal components.

We want to project onto the components that capture most of the variance / information in the data.



Which principal component should we project on?

Anomaly Detection

Define $\mathbf{O} = \mathbf{A} - \mathbf{A}^{(k)}$

The largest rows of $\mathbf{O}$ could be considered anomalies